



## Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 09:21 AM EST

PDB ID : 6OLG  
EMDB ID : EMD-0601  
Title : Human ribosome nascent chain complex stalled by a drug-like small molecule  
(CDH1\_RNC with PP tRNA)  
Authors : Li, W.; Cate, J.H.D.  
Deposited on : 2019-04-16  
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

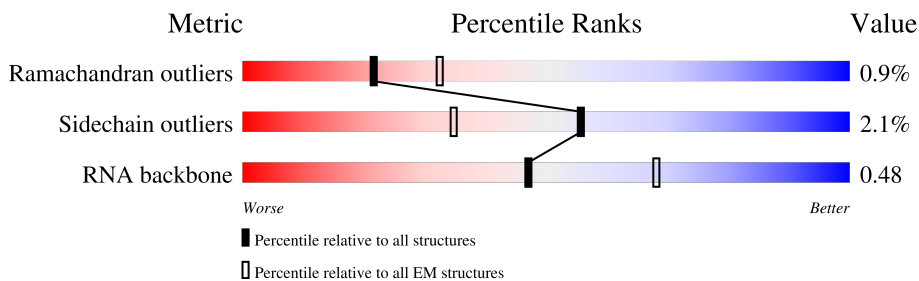
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 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 (#Entries) | EM structures (#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   | AA    | 257    |                  |
| 2   | BA    | 215    |                  |
| 3   | AB    | 394    |                  |
| 4   | BB    | 212    |                  |
| 5   | AC    | 363    |                  |
| 6   | BC    | 222    |                  |
| 7   | A3    | 157    |                  |
| 8   | A4    | 119    |                  |

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| Mol | Chain | Length | Quality of chain        |
|-----|-------|--------|-------------------------|
| 9   | AD    | 294    | 13%<br>94%<br>5%        |
| 10  | AE    | 194    | 25%<br>93%<br>7%        |
| 11  | AF    | 234    | 12%<br>98%              |
| 12  | AG    | 234    | 21%<br>100%             |
| 13  | AH    | 191    | 16%<br>96%              |
| 14  | AI    | 211    | 15%<br>98%              |
| 15  | AJ    | 169    | 21%<br>98%              |
| 16  | AK    | 109    | 99%<br>83%<br>16%       |
| 17  | AL    | 205    | 20%<br>93%<br>5%        |
| 18  | AM    | 139    | 9%<br>99%               |
| 19  | AN    | 203    | 9%<br>99%               |
| 20  | AO    | 195    | 8%<br>98%               |
| 21  | AP    | 153    | 10%<br>100%             |
| 22  | AQ    | 187    | 11%<br>96%              |
| 23  | AR    | 181    | 13%<br>98%              |
| 24  | AS    | 175    | 6%<br>100%              |
| 25  | AT    | 157    | 8%<br>99%               |
| 26  | AU    | 99     | 25%<br>95%<br>5%        |
| 27  | AV    | 129    | 10%<br>100%             |
| 28  | AW    | 121    | 55%<br>98%              |
| 29  | AX    | 117    | 18%<br>99%              |
| 30  | AY    | 127    | 9%<br>99%               |
| 31  | AZ    | 134    | 14%<br>99%              |
| 32  | Aa    | 147    | 9%<br>99%               |
| 33  | Ab    | 121    | 15%<br>50%<br>7%<br>44% |

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| Mol | Chain | Length | Quality of chain       |
|-----|-------|--------|------------------------|
| 34  | Ac    | 103    | 17%<br>93%<br>6%       |
| 35  | Ad    | 106    | 9%<br>100%             |
| 36  | Ae    | 129    | 6%<br>100%             |
| 37  | Af    | 109    | 5%<br>95%<br>5%        |
| 38  | Ag    | 114    | 12%<br>100%            |
| 39  | Ah    | 122    | 15%<br>95%<br>..       |
| 40  | Ai    | 97     | 14%<br>100%            |
| 41  | Aj    | 84     | 5%<br>98%<br>.         |
| 42  | Ak    | 69     | 39%<br>97%<br>.        |
| 43  | Al    | 50     | 10%<br>94%<br>6%       |
| 44  | Am    | 50     | 14%<br>98%<br>.        |
| 45  | An    | 25     | 24%<br>100%            |
| 46  | Ao    | 105    | 20%<br>98%<br>.        |
| 47  | Ap    | 91     | 8%<br>99%<br>.         |
| 48  | Aq    | 138    | 100%<br>92%<br>6%<br>. |
| 49  | At    | 122    | 9%<br>95%<br>5%        |
| 50  | Au    | 217    | 100%<br>93%<br>7%      |
| 51  | A2    | 3612   | 10%<br>71%<br>26%<br>. |
| 52  | B1    | 1708   | 12%<br>71%<br>25%<br>. |
| 53  | BD    | 220    | 62%<br>98%<br>.        |
| 54  | BE    | 257    | 32%<br>98%<br>.        |
| 55  | BF    | 190    | 53%<br>99%<br>.        |
| 56  | BG    | 232    | 51%<br>99%<br>.        |
| 57  | BH    | 183    | 50%<br>99%<br>.        |
| 58  | BI    | 207    | 28%<br>96%<br>.        |

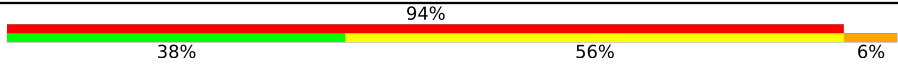
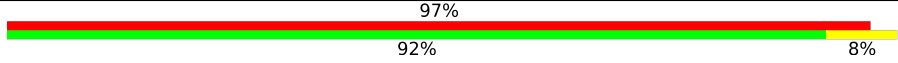
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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|-------------------|
| 59  | BJ    | 179    | 36%<br>97%        |
| 60  | BK    | 98     | 71%<br>96%        |
| 61  | BL    | 153    | 30%<br>98%        |
| 62  | BM    | 120    | 99%<br>100%       |
| 63  | BN    | 149    | 24%<br>99%        |
| 64  | BO    | 136    | 30%<br>98%        |
| 65  | BP    | 120    | 61%<br>90%<br>8%  |
| 66  | BQ    | 139    | 52%<br>99%        |
| 67  | BR    | 125    | 55%<br>98%        |
| 68  | BS    | 139    | 58%<br>94%        |
| 69  | BT    | 143    | 53%<br>98%        |
| 70  | BU    | 97     | 59%<br>100%       |
| 71  | BV    | 81     | 41%<br>98%        |
| 72  | BW    | 129    | 15%<br>96%        |
| 73  | BX    | 139    | 20%<br>96%        |
| 74  | BY    | 125    | 38%<br>99%        |
| 75  | BZ    | 86     | 70%<br>98%        |
| 76  | Ba    | 97     | 25%<br>100%       |
| 77  | Bb    | 80     | 42%<br>99%        |
| 78  | Bc    | 62     | 53%<br>97%        |
| 79  | Bd    | 51     | 35%<br>96%        |
| 80  | Be    | 55     | 44%<br>95%<br>5%  |
| 81  | Bf    | 73     | 96%<br>99%        |
| 82  | Bg    | 314    | 85%<br>99%        |
| 83  | Bv    | 76     | 58%<br>62%<br>36% |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 84  | Bx    | 16     |  <p>94%</p> <p>38% 56% 6%</p> |
| 85  | A     | 39     |  <p>97%</p> <p>92% 8%</p>     |

## 2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 216796 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 1   | AA    | 252      | 1930  | 1209 | 395 | 320 | 6 | 0       | 0     |

- Molecule 2 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 2   | BA    | 215      | 1704  | 1083 | 298 | 315 | 8 | 0       | 0     |

- Molecule 3 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 3   | AB    | 394      | 3178  | 2024 | 596 | 544 | 14 | 0       | 0     |

- Molecule 4 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 4   | BB    | 212      | 1722  | 1093 | 308 | 307 | 14 | 0       | 0     |

- Molecule 5 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 5   | AC    | 363      | 2888  | 1817 | 577 | 480 | 14 | 0       | 0     |

- Molecule 6 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 6   | BC    | 222      | 1724  | 1114 | 296 | 304 | 10 | 0       | 0     |

- Molecule 7 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
|     |       |          | Total | C    | N   | O    | P   |         |       |
| 7   | A3    | 157      | 3337  | 1489 | 587 | 1104 | 157 | 0       | 0     |

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
|     |       |          | Total | C    | N   | O   | P   |         |       |
| 8   | A4    | 119      | 2541  | 1132 | 454 | 836 | 119 | 0       | 0     |

- Molecule 9 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 9   | AD    | 294      | 2392  | 1510 | 436 | 432 | 14 | 0       | 0     |

- Molecule 10 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 10  | AE    | 194      | 1571  | 1013 | 294 | 263 | 1 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 11  | AF    | 234      | 1950  | 1252 | 376 | 313 | 9 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 12  | AG    | 234      | 1880  | 1197 | 362 | 317 | 4 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 13  | AH    | 191      | 1526  | 960 | 285 | 275 | 6 | 0       | 0     |

- Molecule 14 is a protein called 60S ribosomal protein L10.



| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 14  | AI    | 208      | 1692  | 1074 | 327 | 278 | 13 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 15  | AJ    | 169      | 1353  | 855 | 252 | 240 | 6 | 0       | 0     |

- Molecule 16 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 16  | AK    | 109      | 872   | 554 | 159 | 151 | 8 | 0       | 0     |

- Molecule 17 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 17  | AL    | 205      | 1657  | 1036 | 344 | 273 | 4 | 0       | 0     |

- Molecule 18 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 18  | AM    | 139      | 1138  | 730 | 218 | 183 | 7 | 0       | 0     |

- Molecule 19 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 19  | AN    | 203      | 1701  | 1072 | 359 | 266 | 4 | 0       | 0     |

- Molecule 20 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 20  | AO    | 195      | 1606  | 1034 | 315 | 252 | 5 | 0       | 0     |

- Molecule 21 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | AP    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 776 | 241 | 216 | 9 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | AQ    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1513  | 944 | 314 | 250 | 5 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | AR    | 181      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1517  | 938 | 329 | 241 | 9 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 24  | AS    | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1449  | 921 | 283 | 234 | 11 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | AT    | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1284  | 815 | 250 | 214 | 5 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | AU    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 808   | 518 | 141 | 147 | 2 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | AV    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 613 | 182 | 169 | 5 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 28  | AW    | 121      | 989   | 617 | 202 | 167 | 3 | 0       | 0     |

- Molecule 29 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 29  | AX    | 117      | 958   | 612 | 180 | 165 | 1 | 0       | 0     |

- Molecule 30 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 30  | AY    | 127      | 1064  | 668 | 216 | 177 | 3 | 0       | 0     |

- Molecule 31 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 31  | AZ    | 134      | 1103  | 712 | 207 | 181 | 3 | 0       | 0     |

- Molecule 32 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 32  | Aa    | 147      | 1162  | 736 | 237 | 186 | 3 | 0       | 0     |

- Molecule 33 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
|     |       |          | Total | C   | N   | O  | S |         |       |
| 33  | Ab    | 68       | 559   | 344 | 122 | 90 | 3 | 0       | 0     |

- Molecule 34 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 34  | Ac    | 103      | 801   | 508 | 141 | 145 | 7 | 0       | 0     |

- Molecule 35 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 35  | Ad    | 106      | 879   | 555 | 170 | 152 | 2 | 0       | 0     |

- Molecule 36 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 36  | Ae    | 129      | 1064  | 673 | 220 | 166 | 5 | 0       | 0     |

- Molecule 37 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 37  | Af    | 109      | 876   | 555 | 174 | 144 | 3 | 0       | 0     |

- Molecule 38 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 38  | Ag    | 114      | 906   | 566 | 187 | 147 | 6 | 0       | 0     |

- Molecule 39 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 39  | Ah    | 122      | 1015  | 641 | 205 | 168 | 1 | 0       | 0     |

- Molecule 40 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 40  | Ai    | 97       | 794   | 497 | 168 | 124 | 5 | 0       | 0     |

- Molecule 41 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 41  | Aj    | 84       | 689   | 423 | 152 | 109 | 5 | 0       | 0     |

- Molecule 42 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
|     |       |          | Total | C   | N   | O  | S |         |       |
| 42  | Ak    | 69       | 569   | 366 | 103 | 99 | 1 | 0       | 0     |

- Molecule 43 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 43  | Al    | 50       | 444   | 281 | 98 | 64 | 1 | 0       | 0     |

- Molecule 44 is a protein called 60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 44  | Am    | 50       | 411   | 254 | 87 | 64 | 6 | 0       | 0     |

- Molecule 45 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 45  | An    | 25       | 240   | 145 | 64 | 28 | 3 | 0       | 0     |

- Molecule 46 is a protein called 60S ribosomal protein L36a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 46  | Ao    | 105      | 863   | 542 | 175 | 140 | 6 | 0       | 0     |

- Molecule 47 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 47  | Ap    | 91       | 708   | 445 | 136 | 120 | 7 | 0       | 0     |

- Molecule 48 is a protein called 60S ribosomal protein L12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 48  | Aq    | 138      | 1046  | 654 | 196 | 193 | 3 | 0       | 0     |

- Molecule 49 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | At    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 980   | 607 | 204 | 165 | 4 |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L10a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | Au    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1744  | 1114 | 314 | 307 | 9 |         |       |

- Molecule 51 is a RNA chain called 28S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 51  | A2    | 3612     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 77427 | 34482 | 14158 | 25175 | 3612 |         |       |

- Molecule 52 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 52  | B1    | 1708     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36456 | 16274 | 6546 | 11928 | 1708 |         |       |

- Molecule 53 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 53  | BD    | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1709  | 1090 | 308 | 304 | 7 |         |       |

- Molecule 54 is a protein called 40S ribosomal protein S4, Y isoform 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 54  | BE    | 257      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2031  | 1298 | 381 | 344 | 8 |         |       |

- Molecule 55 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | BF    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1502  | 939 | 285 | 271 | 7 |         |       |

- Molecule 56 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 56  | BG    | 232      | 1884  | 1176 | 379 | 322 | 7 | 0       | 0     |

- Molecule 57 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 57  | BH    | 183      | 1479  | 941 | 272 | 265 | 1 | 0       | 0     |

- Molecule 58 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 58  | BI    | 207      | 1696  | 1064 | 334 | 293 | 5 | 0       | 0     |

- Molecule 59 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 59  | BJ    | 179      | 1495  | 953 | 299 | 241 | 2 | 0       | 0     |

- Molecule 60 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 60  | BK    | 98       | 827   | 539 | 148 | 134 | 6 | 0       | 0     |

- Molecule 61 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 61  | BL    | 153      | 1258  | 804 | 235 | 213 | 6 | 0       | 0     |

- Molecule 62 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 62  | BM    | 120      | 931   | 584 | 164 | 174 | 9 | 0       | 0     |

- Molecule 63 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 63  | BN    | 149      | 1202  | 770 | 228 | 203 | 1 | 0       | 0     |

- Molecule 64 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 64  | BO    | 136      | 1016  | 621 | 199 | 190 | 6 | 0       | 0     |

- Molecule 65 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 65  | BP    | 120      | 999   | 636 | 188 | 168 | 7 | 0       | 0     |

- Molecule 66 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 66  | BQ    | 139      | 1109  | 704 | 210 | 192 | 3 | 0       | 0     |

- Molecule 67 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 67  | BR    | 125      | 1011  | 634 | 187 | 186 | 4 | 0       | 0     |

- Molecule 68 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 68  | BS    | 139      | 1154  | 725 | 233 | 195 | 1 | 0       | 0     |

- Molecule 69 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 69  | BT    | 143      | 1112  | 697 | 214 | 198 | 3 | 0       | 0     |

- Molecule 70 is a protein called 40S ribosomal protein S20.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 70  | BU    | 97       | 769   | 483 | 144 | 138 | 4 | 0       | 0     |

- Molecule 71 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 71  | BV    | 81       | 617   | 380 | 114 | 118 | 5 | 0       | 0     |

- Molecule 72 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 72  | BW    | 129      | 1034  | 659 | 193 | 176 | 6 | 0       | 0     |

- Molecule 73 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 73  | BX    | 139      | 1080  | 682 | 214 | 181 | 3 | 0       | 0     |

- Molecule 74 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 74  | BY    | 125      | 1015  | 642 | 199 | 169 | 5 | 0       | 0     |

- Molecule 75 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 75  | BZ    | 86       | 688   | 442 | 129 | 116 | 1 | 0       | 0     |

- Molecule 76 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 76  | Ba    | 97       | 774   | 481 | 160 | 128 | 5 | 0       | 0     |

- Molecule 77 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | Bb    | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 391 | 116 | 111 | 7 |         |       |

- Molecule 78 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 78  | Bc    | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 488   | 297 | 97 | 92 | 2 |         |       |

- Molecule 79 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 79  | Bd    | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 427   | 269 | 87 | 66 | 5 |         |       |

- Molecule 80 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 80  | Be    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 437   | 272 | 96 | 68 | 1 |         |       |

- Molecule 81 is a protein called 40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81  | Bf    | 73       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 601   | 379 | 115 | 100 | 7 |         |       |

- Molecule 82 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 82  | Bg    | 314      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2440  | 1537 | 425 | 466 | 12 |         |       |

- Molecule 83 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 83  | Bv    | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1623  | 723 | 290 | 534 | 76 |         |       |

- Molecule 84 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
|     |       |          | Total | C   | N  | O   | P  |         |       |
| 84  | Bx    | 16       | 320   | 144 | 32 | 128 | 16 | 0       | 0     |

- Molecule 85 is a protein called Cadherin-1.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
|     |       |          | Total | C   | N  | O  |         |       |
| 85  | A     | 39       | 190   | 112 | 39 | 39 | 0       | 0     |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| A     | 6       | ALA      | -      | insertion | UNP P12830 |
| A     | 10      | GLU      | VAL    | conflict  | UNP P12830 |

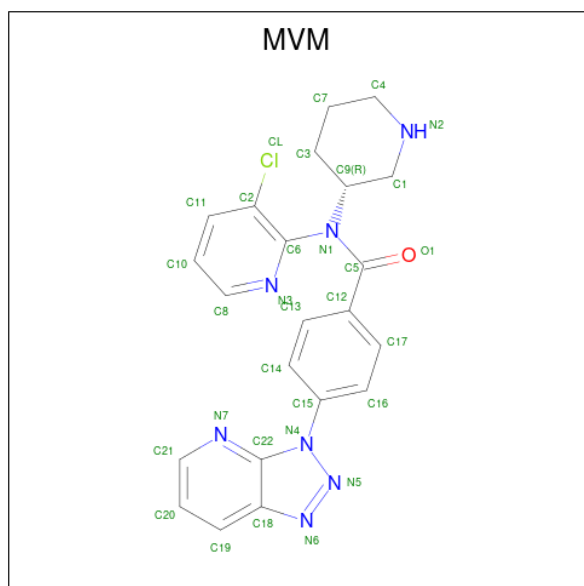
- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
|     |       |          | Total | Mg  |         |
| 86  | AB    | 2        | 2     | 2   | 0       |
| 86  | A3    | 6        | 6     | 6   | 0       |
| 86  | A4    | 9        | 9     | 9   | 0       |
| 86  | AP    | 1        | 1     | 1   | 0       |
| 86  | AY    | 1        | 1     | 1   | 0       |
| 86  | Aa    | 1        | 1     | 1   | 0       |
| 86  | Ae    | 1        | 1     | 1   | 0       |
| 86  | A2    | 226      | 226   | 226 | 0       |
| 86  | B1    | 75       | 75    | 75  | 0       |
| 86  | BI    | 1        | 1     | 1   | 0       |
| 86  | Ba    | 1        | 1     | 1   | 0       |
| 86  | Bv    | 2        | 2     | 2   | 0       |

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 87  | Aj    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | Ao    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | Ap    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | Ba    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | Bd    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 88 is N-(3-chloropyridin-2-yl)-N-[(3R)-piperidin-3-yl]-4-(3H-[1,2,3]triazolo[4,5-b]pyridin-3-yl)benzamide (three-letter code: MVM) (formula: C<sub>22</sub>H<sub>20</sub>ClN<sub>7</sub>O).

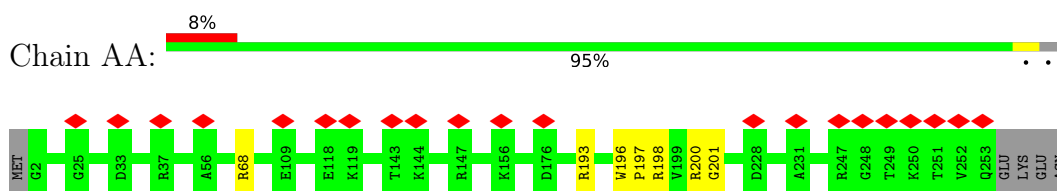


| Mol | Chain | Residues | Atoms |    |    |   | AltConf |   |
|-----|-------|----------|-------|----|----|---|---------|---|
| 88  | A2    | 1        | Total | C  | Cl | N | O       | 0 |
|     |       |          | 31    | 22 | 1  | 7 | 1       |   |

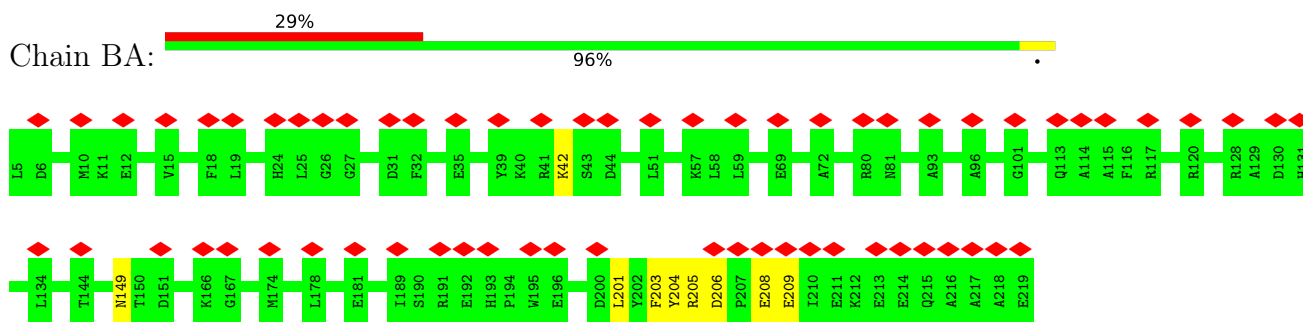
### 3 Residue-property plots [i](#)

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

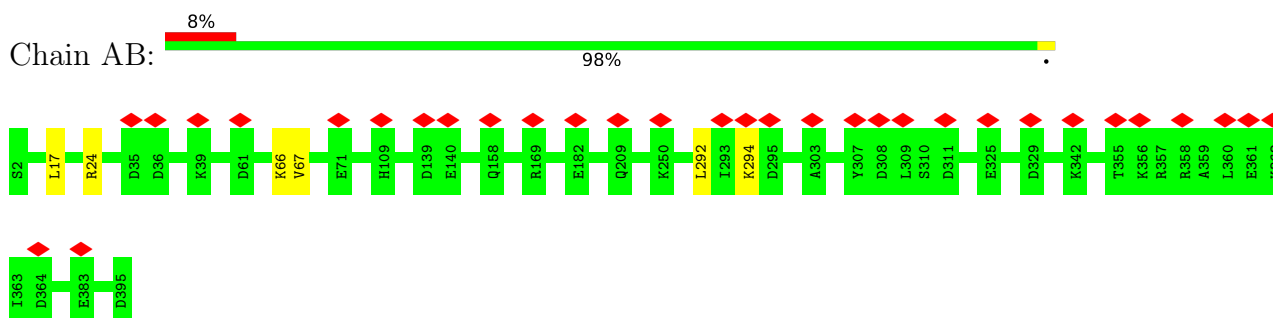
- Molecule 1: 60S ribosomal protein L8



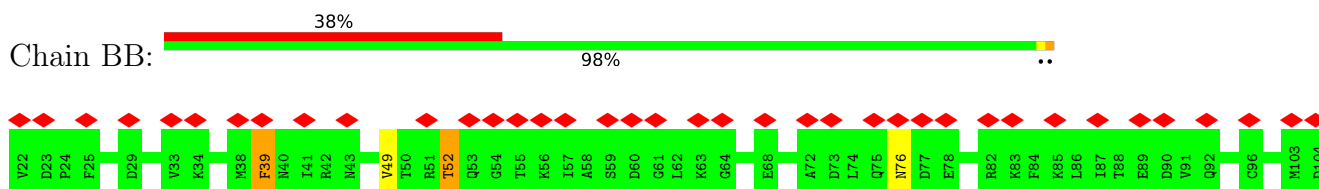
- Molecule 2: 40S ribosomal protein SA

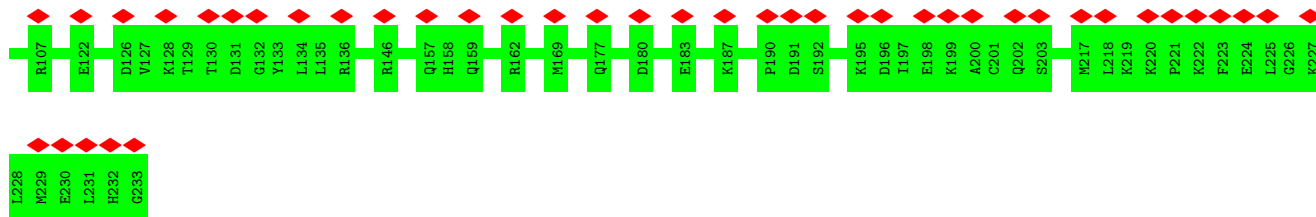


- Molecule 3: 60S ribosomal protein L3

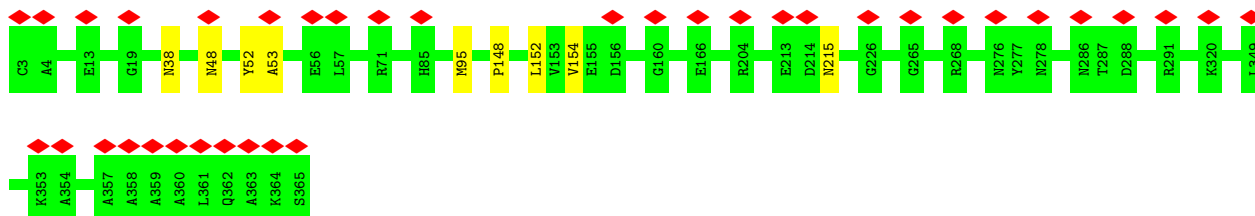


- Molecule 4: 40S ribosomal protein S3a

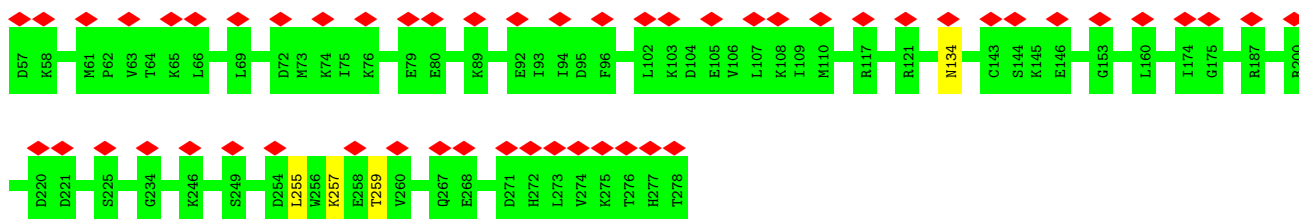




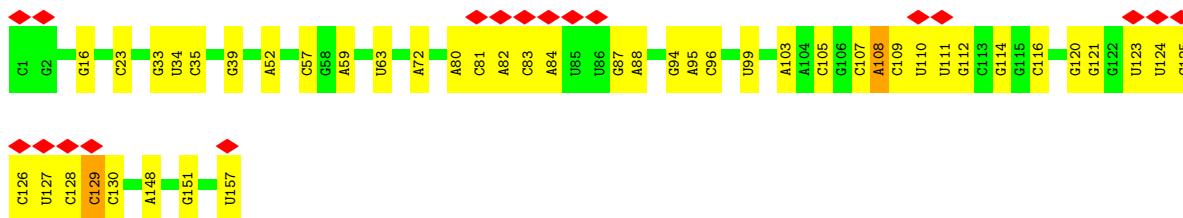
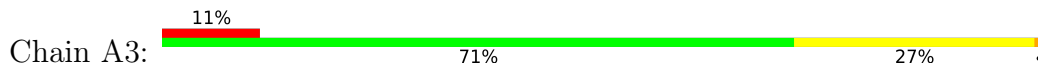
• Molecule 5: 60S ribosomal protein L4



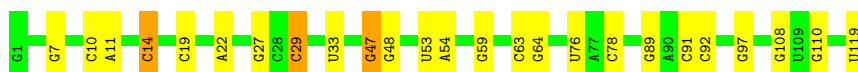
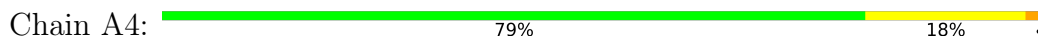
• Molecule 6: 40S ribosomal protein S2



• Molecule 7: 5.8S ribosomal RNA

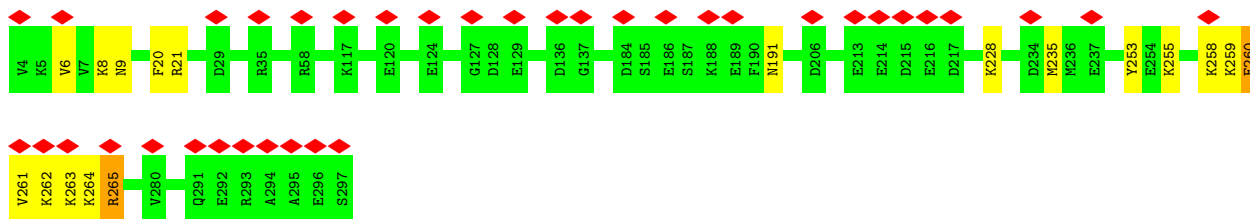


• Molecule 8: 5S ribosomal RNA



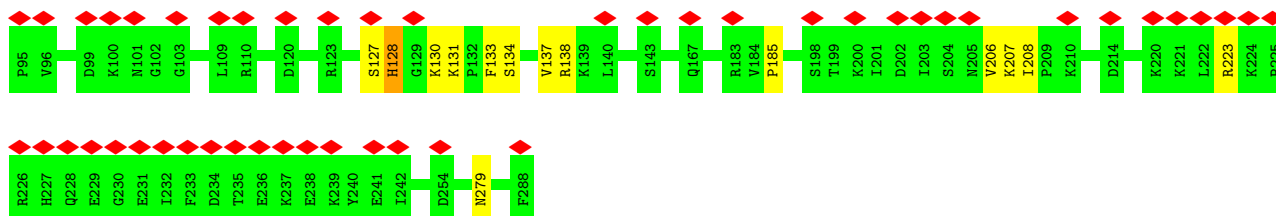
• Molecule 9: 60S ribosomal protein L5

Chain AD: 



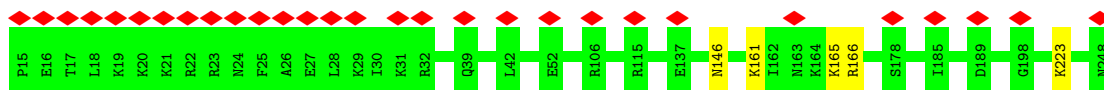
• Molecule 10: 60S ribosomal protein L6

Chain AE: 



• Molecule 11: 60S ribosomal protein L7

Chain AF: 



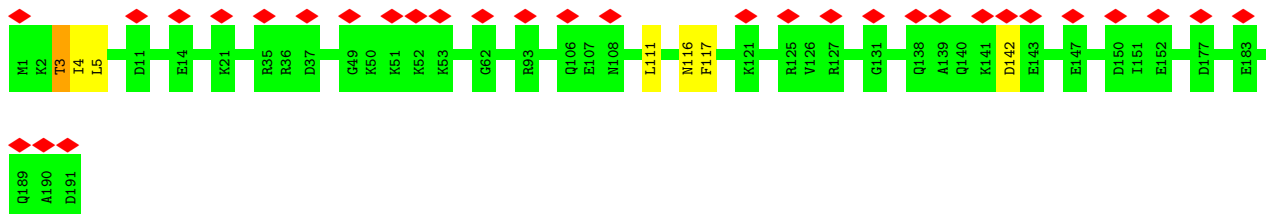
• Molecule 12: 60S ribosomal protein L7a

Chain AG: 

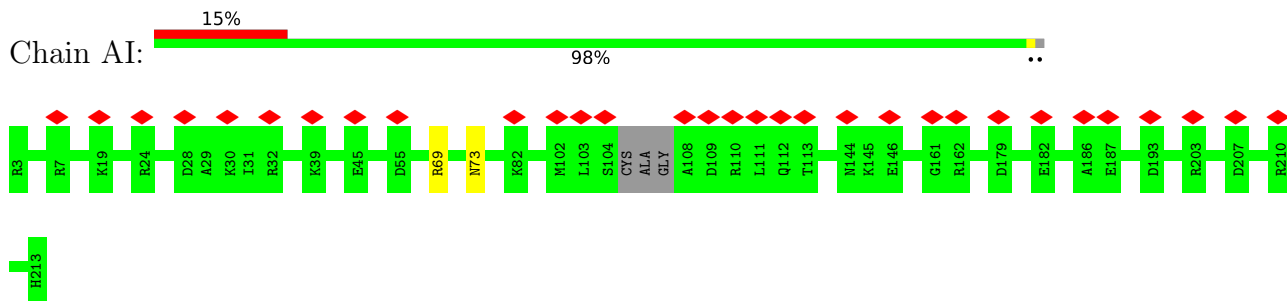


• Molecule 13: 60S ribosomal protein L9

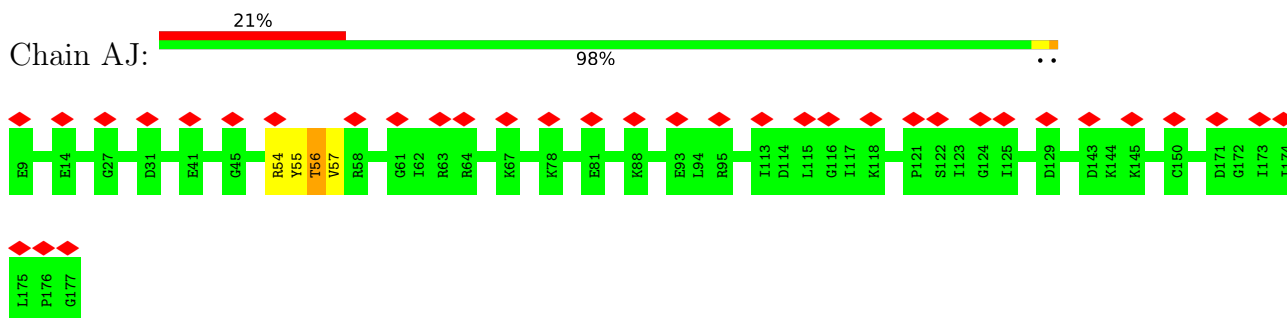
Chain AH: 



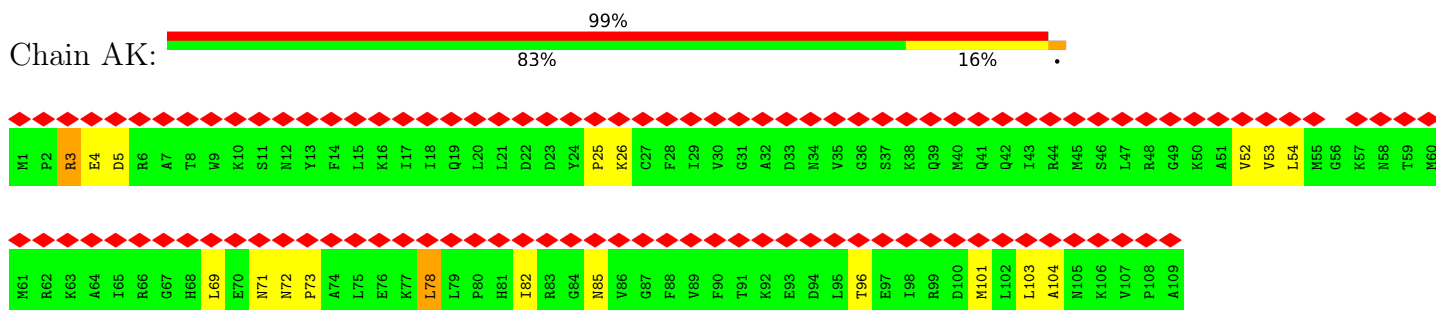
- Molecule 14: 60S ribosomal protein L10



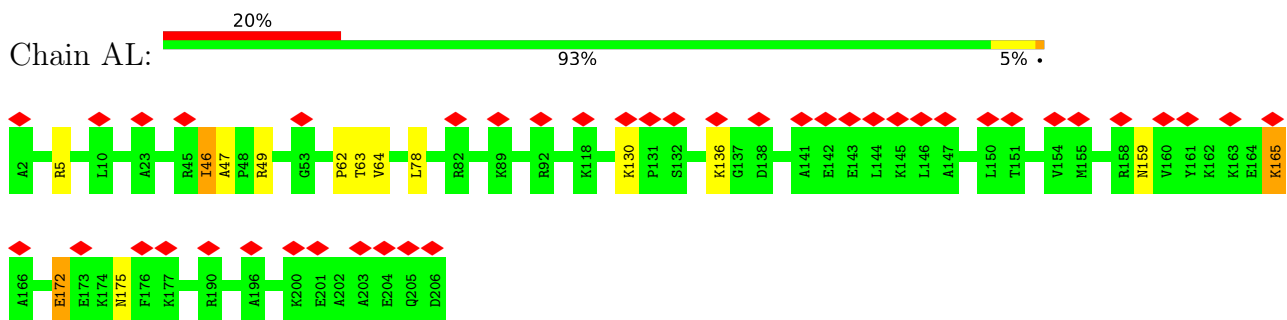
- Molecule 15: 60S ribosomal protein L11



- Molecule 16: 60S acidic ribosomal protein P0



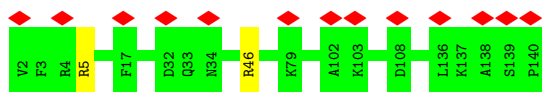
- Molecule 17: 60S ribosomal protein L13



- Molecule 18: 60S ribosomal protein L14

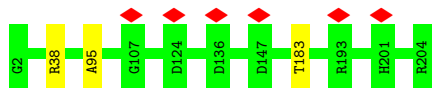






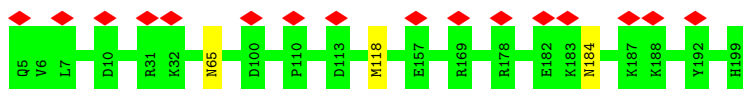
- Molecule 19: 60S ribosomal protein L15

Chain AN: 99%



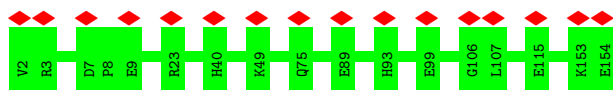
- Molecule 20: 60S ribosomal protein L13a

Chain AO: 98%



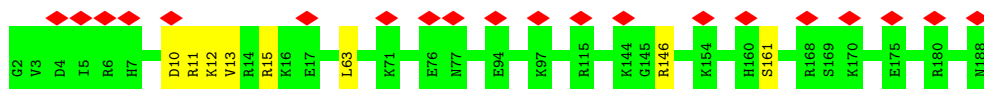
- Molecule 21: 60S ribosomal protein L17

Chain AP: 100%



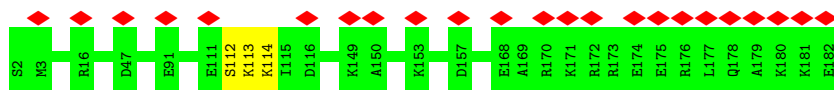
- Molecule 22: 60S ribosomal protein L18

Chain AQ: 96%



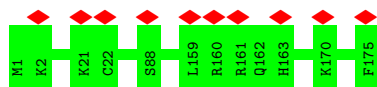
- Molecule 23: 60S ribosomal protein L19

Chain AR: 98%

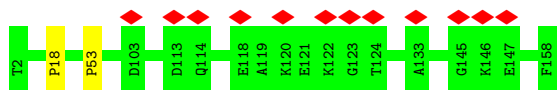


- Molecule 24: 60S ribosomal protein L18a

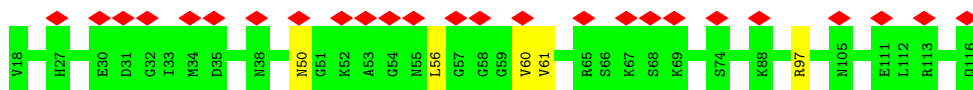
Chain AS: 100%



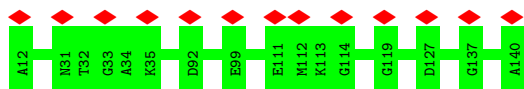
- Molecule 25: 60S ribosomal protein L21



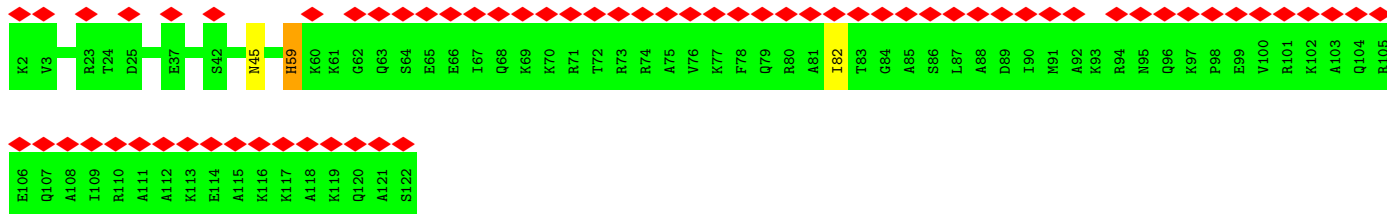
- Molecule 26: 60S ribosomal protein L22



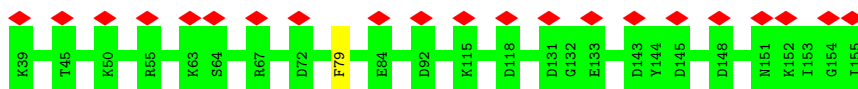
- Molecule 27: 60S ribosomal protein L23



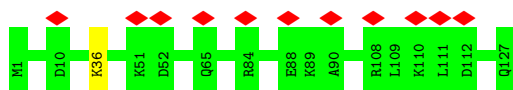
- Molecule 28: 60S ribosomal protein L24



- Molecule 29: 60S ribosomal protein L23a

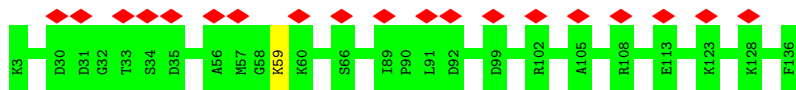


- Molecule 30: 60S ribosomal protein L26

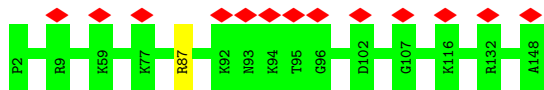


- Molecule 31: 60S ribosomal protein L27

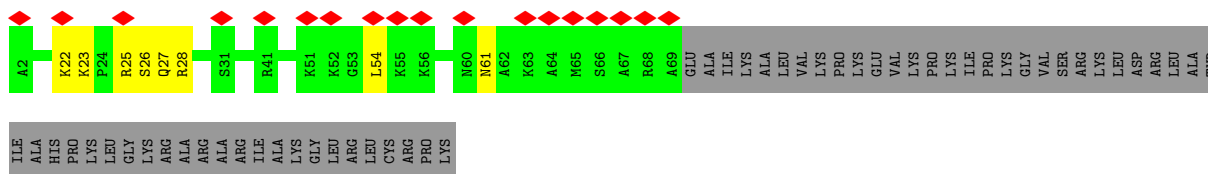




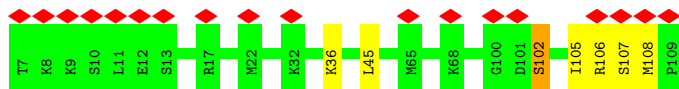
• Molecule 32: 60S ribosomal protein L27a



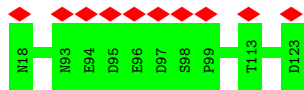
• Molecule 33: 60S ribosomal protein L29



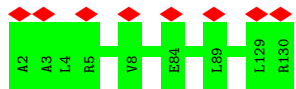
• Molecule 34: 60S ribosomal protein L30



• Molecule 35: 60S ribosomal protein L31

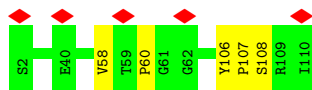


• Molecule 36: 60S ribosomal protein L32

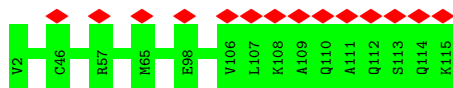


• Molecule 37: 60S ribosomal protein L35a





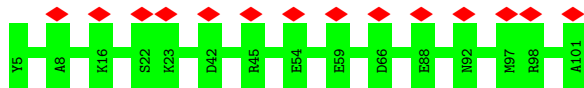
- Molecule 38: 60S ribosomal protein L34



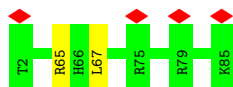
- Molecule 39: 60S ribosomal protein L35



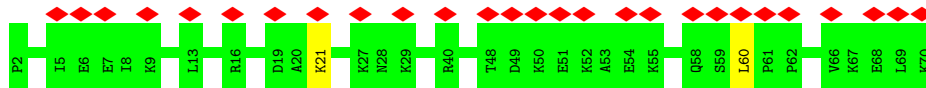
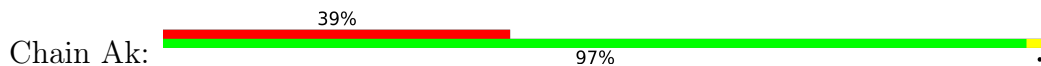
- Molecule 40: 60S ribosomal protein L36



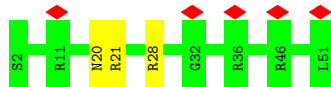
- Molecule 41: 60S ribosomal protein L37



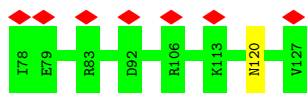
- Molecule 42: 60S ribosomal protein L38



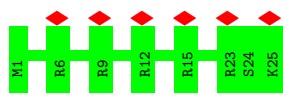
- Molecule 43: 60S ribosomal protein L39



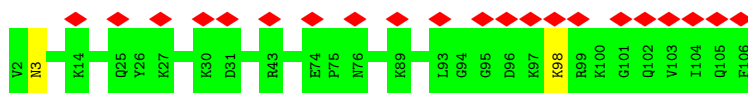
- Molecule 44: 60S ribosomal protein L40



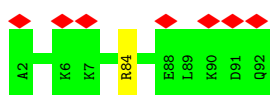
• Molecule 45: 60S ribosomal protein L41



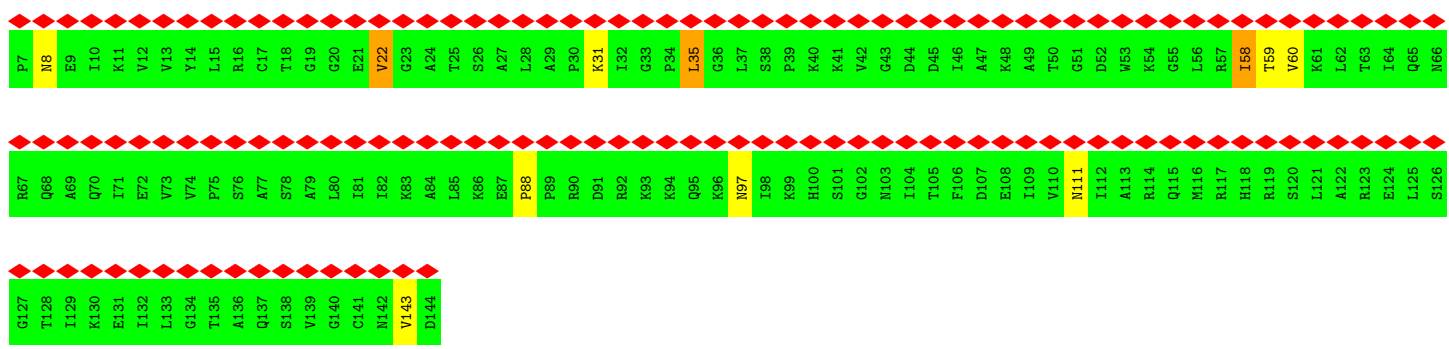
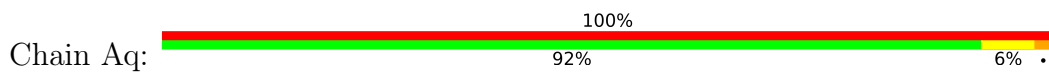
• Molecule 46: 60S ribosomal protein L36a



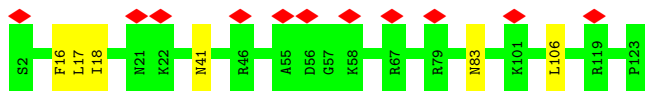
• Molecule 47: 60S ribosomal protein L37a



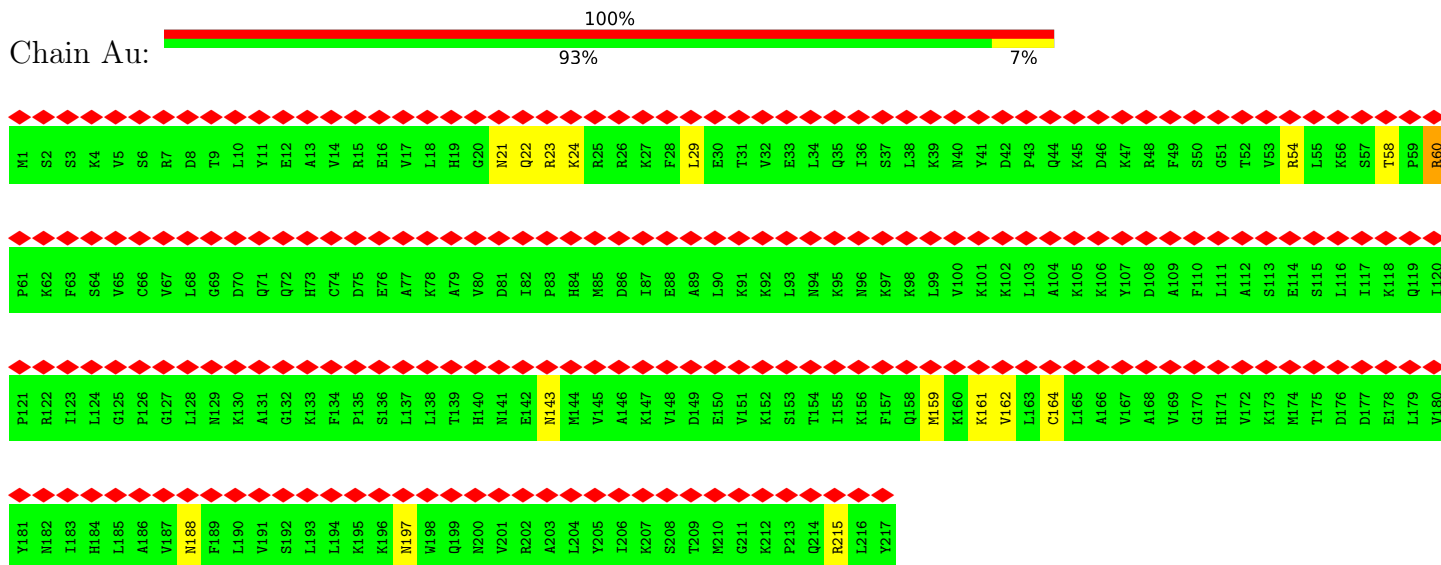
• Molecule 48: 60S ribosomal protein L12



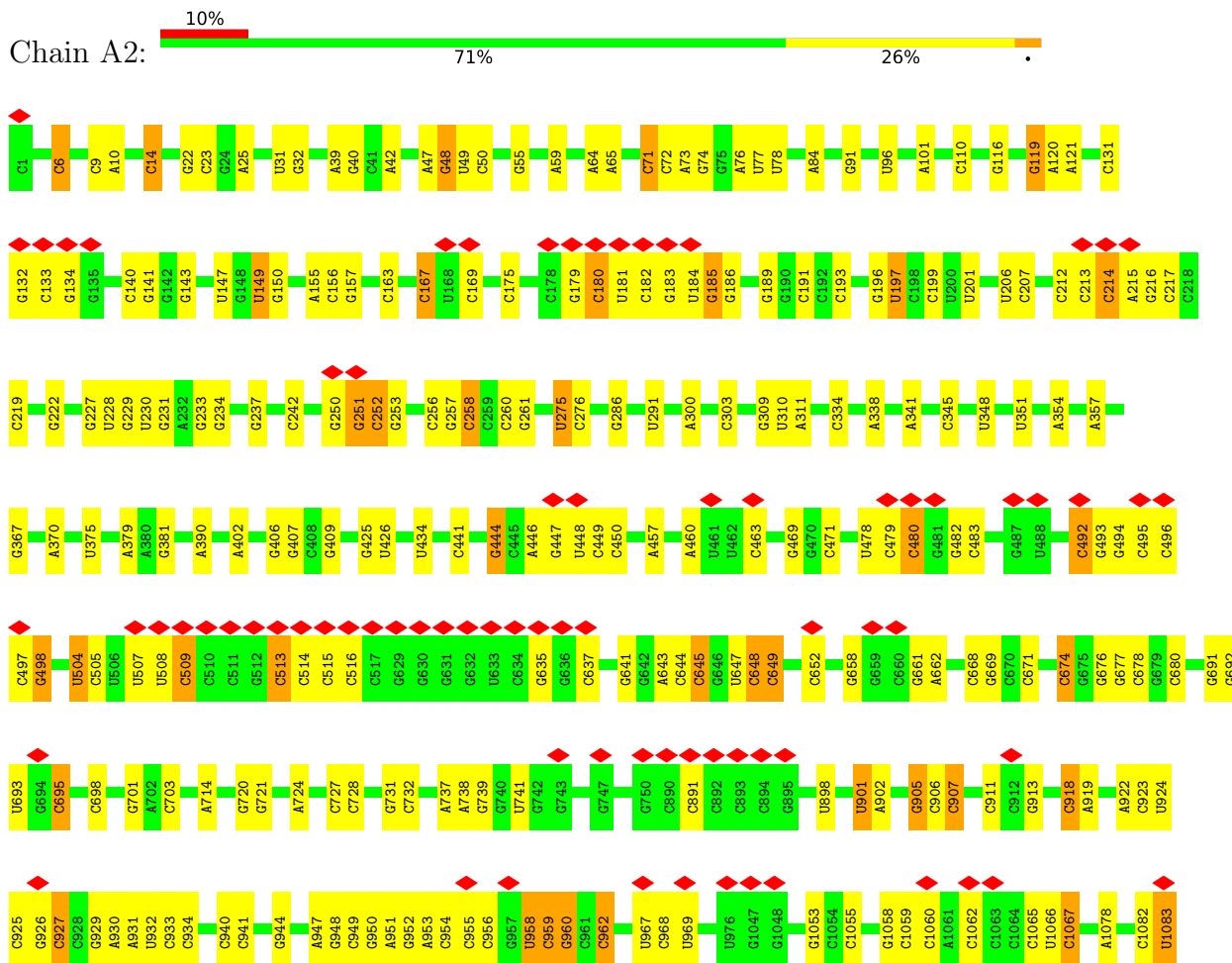
• Molecule 49: 60S ribosomal protein L28



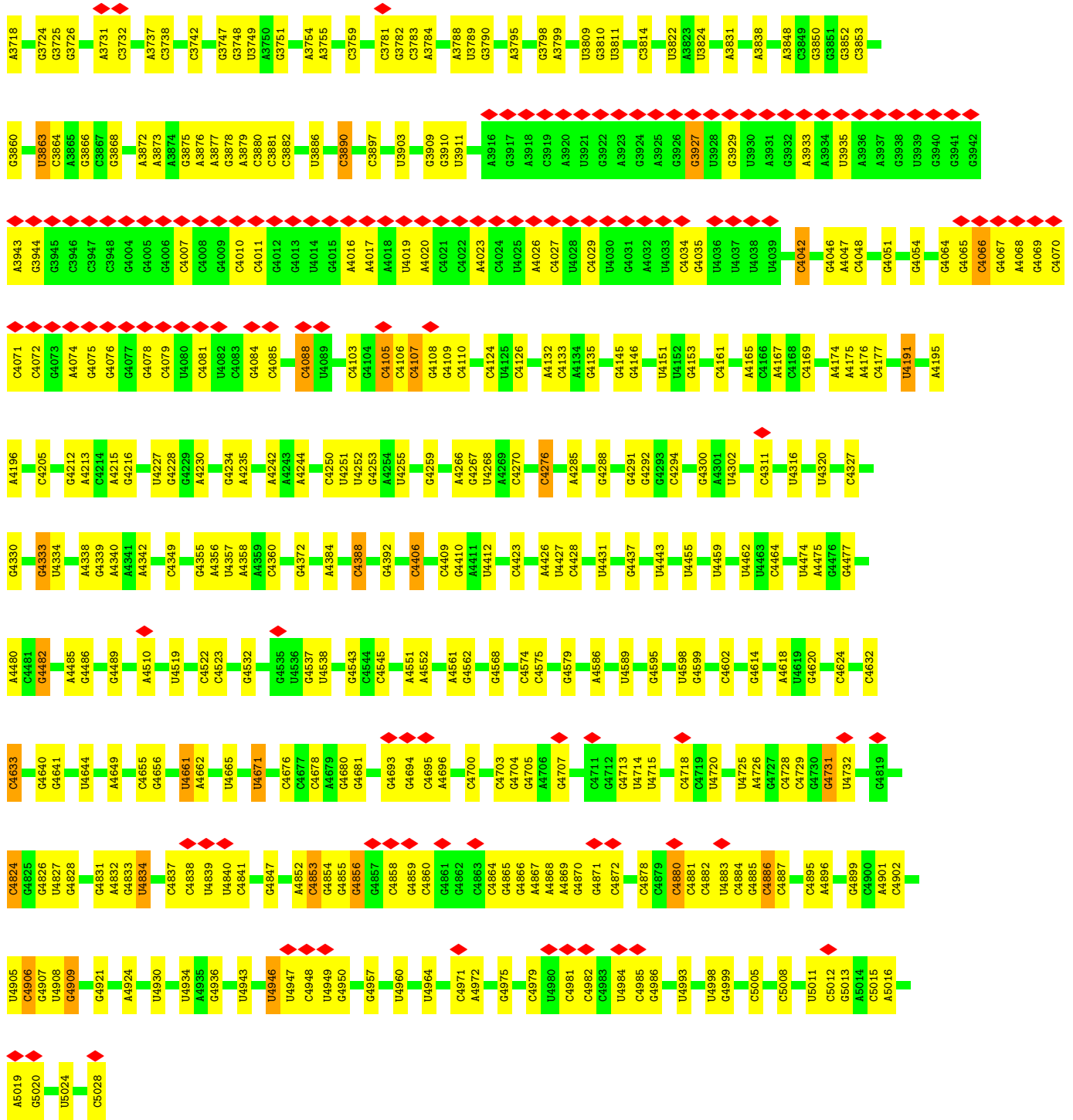
• Molecule 50: 60S ribosomal protein L10a



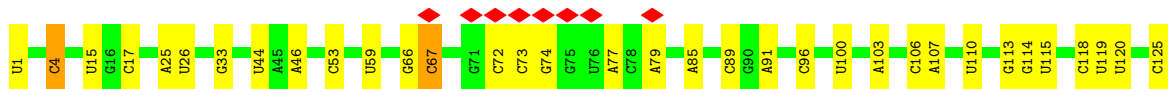
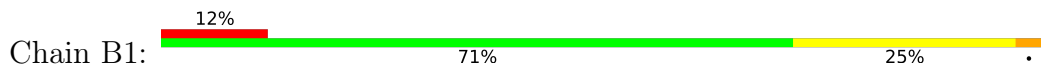
• Molecule 51: 28S ribosomal RNA



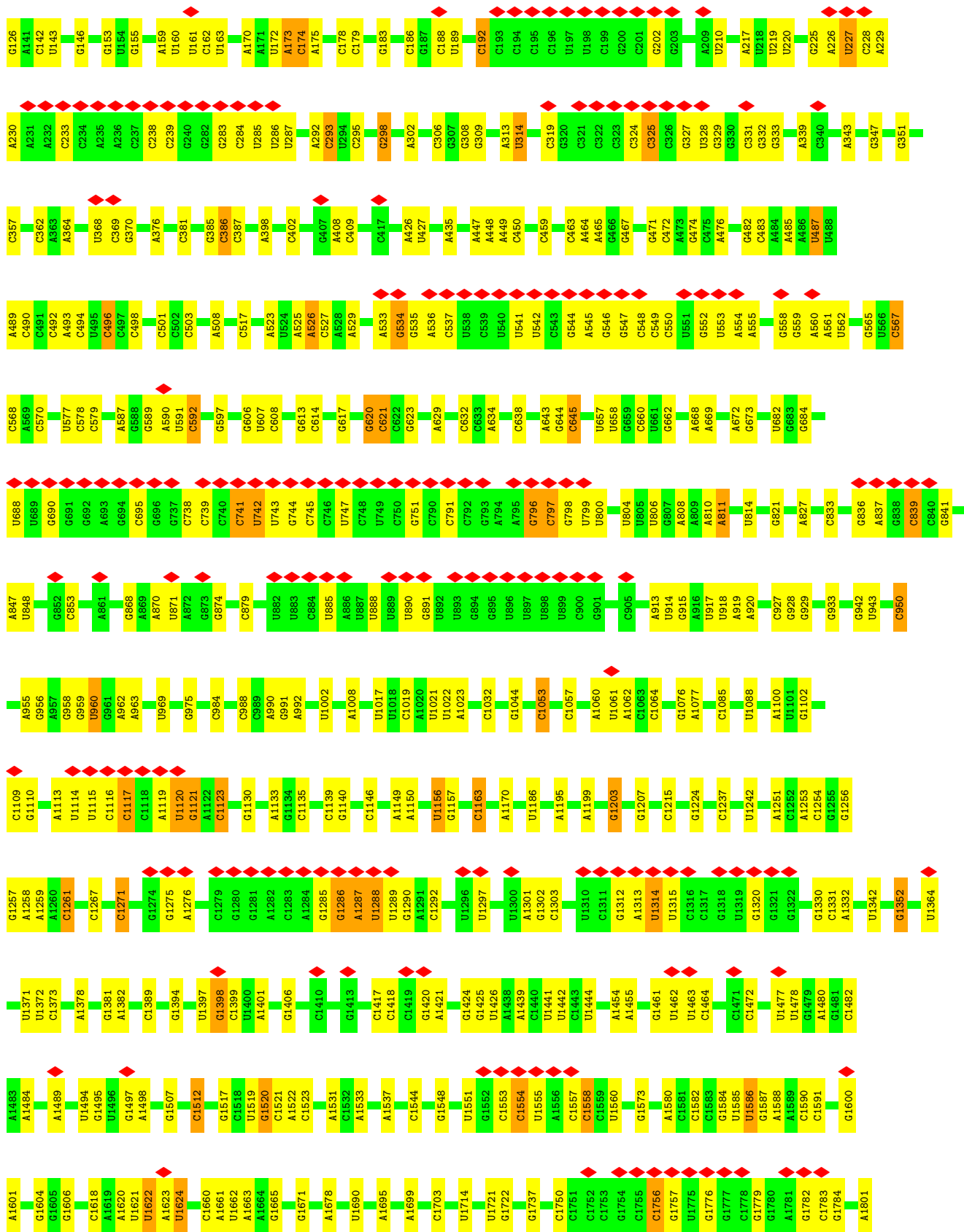


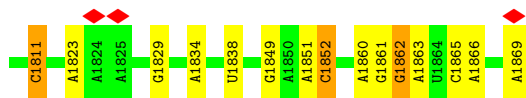


● Molecule 52: 18S ribosomal RNA

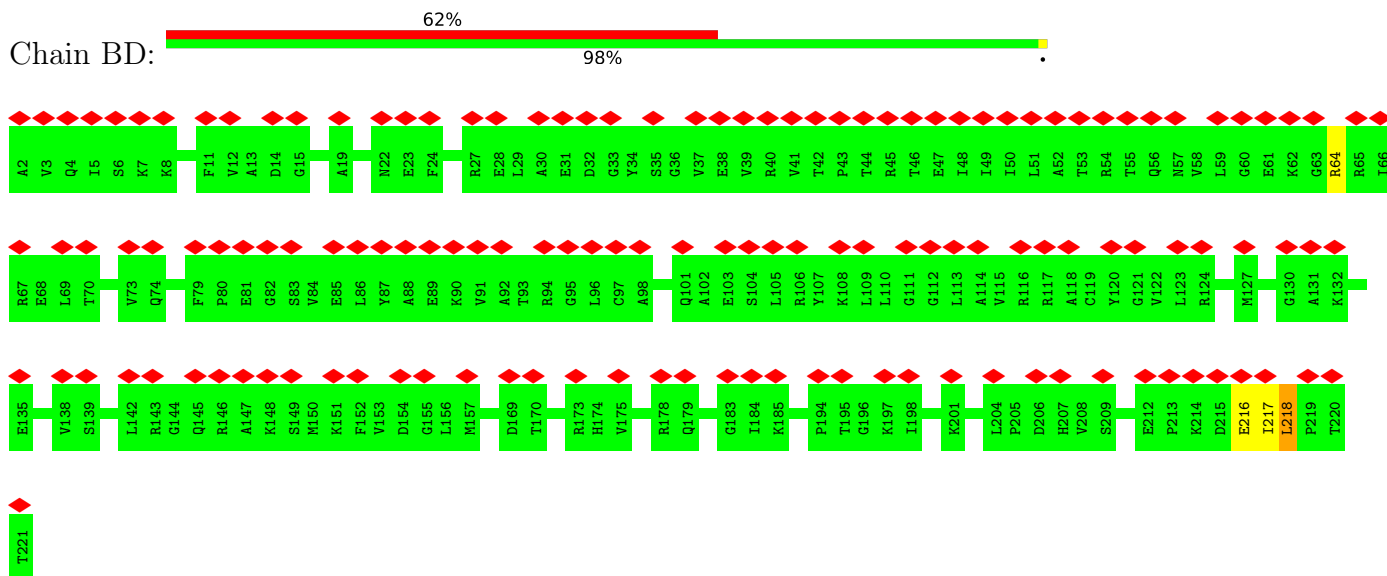




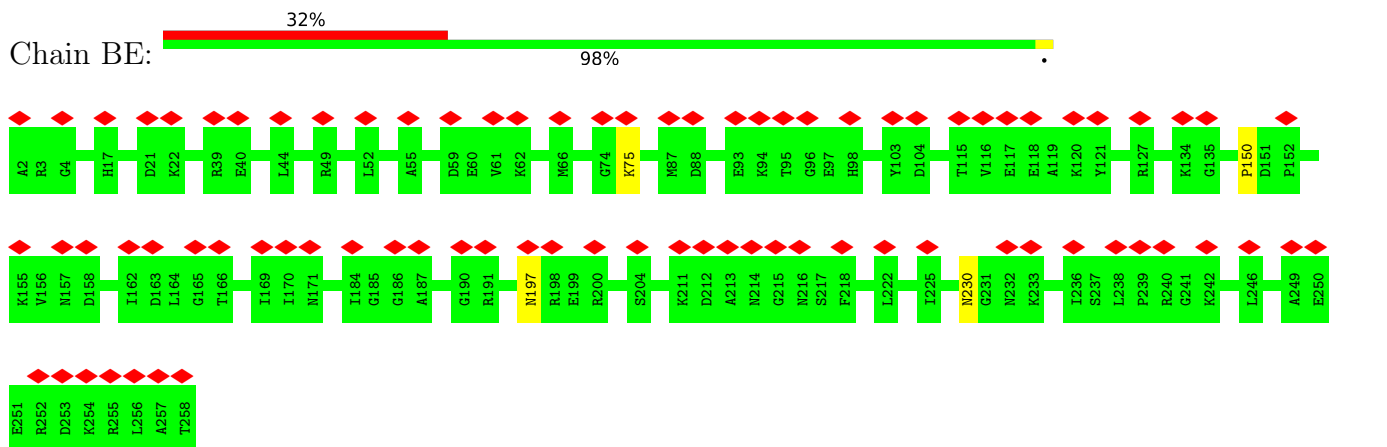




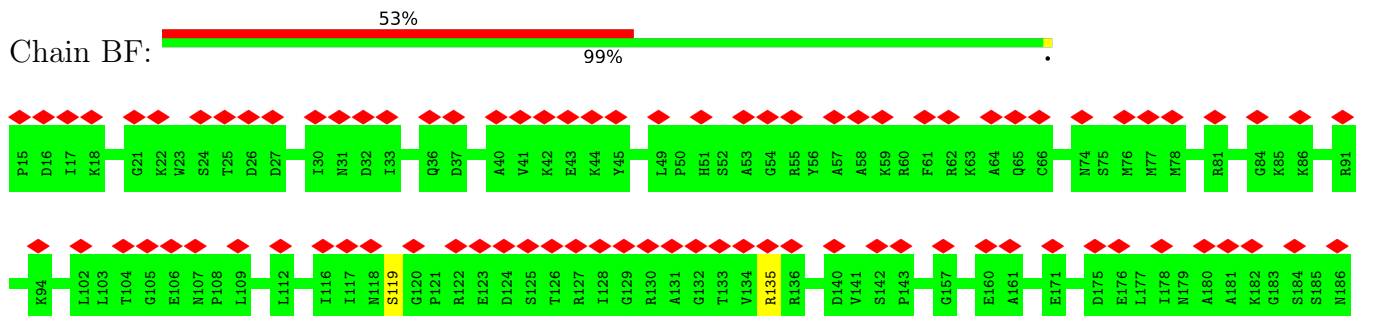
- Molecule 53: 40S ribosomal protein S3

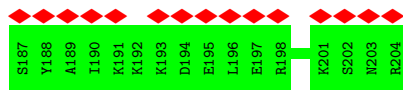


- Molecule 54: 40S ribosomal protein S4, Y isoform 1



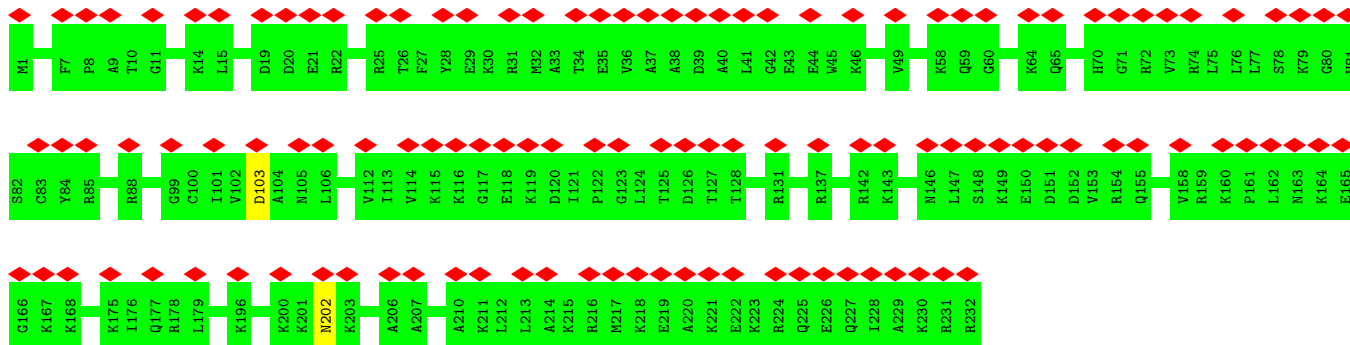
- Molecule 55: 40S ribosomal protein S5





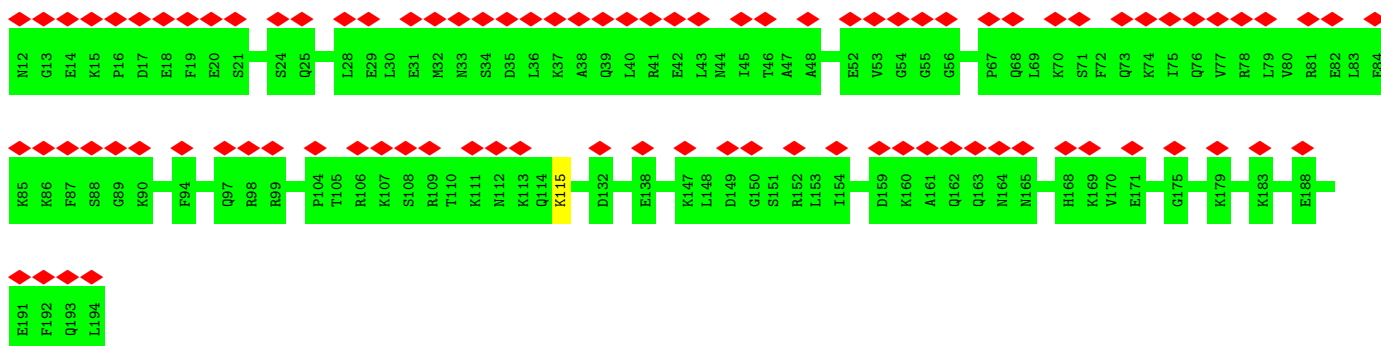
- Molecule 56: 40S ribosomal protein S6

Chain BG: 51% 99%



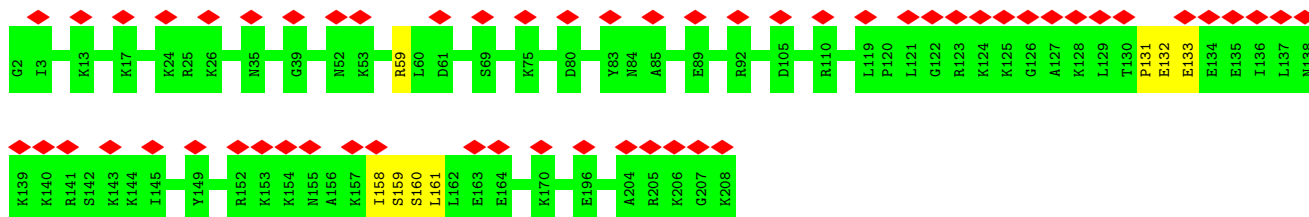
- Molecule 57: 40S ribosomal protein S7

Chain BH: 50% 99%



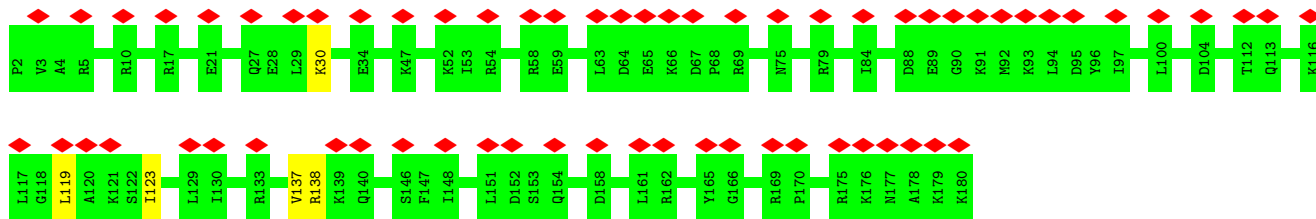
- Molecule 58: 40S ribosomal protein S8

Chain BI: 28% 96%

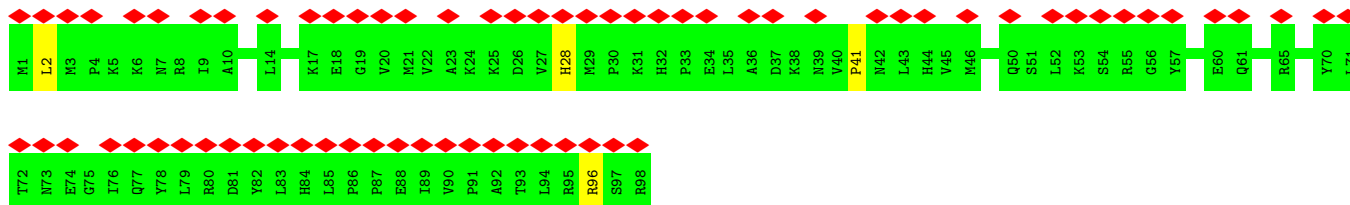
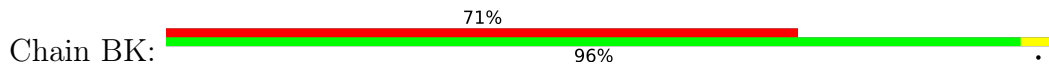


- Molecule 59: 40S ribosomal protein S9

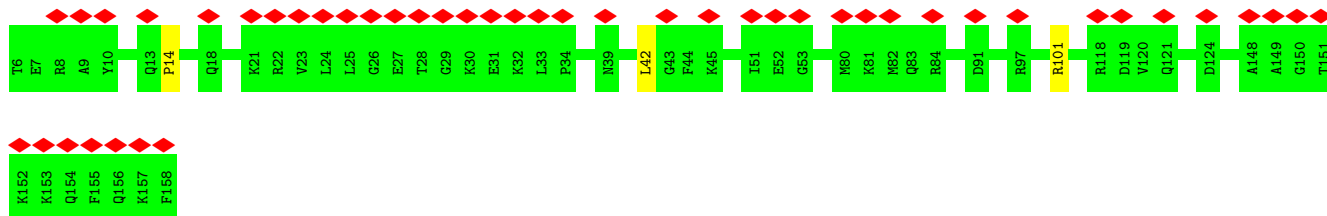
Chain BJ: 36% 97%



• Molecule 60: 40S ribosomal protein S10



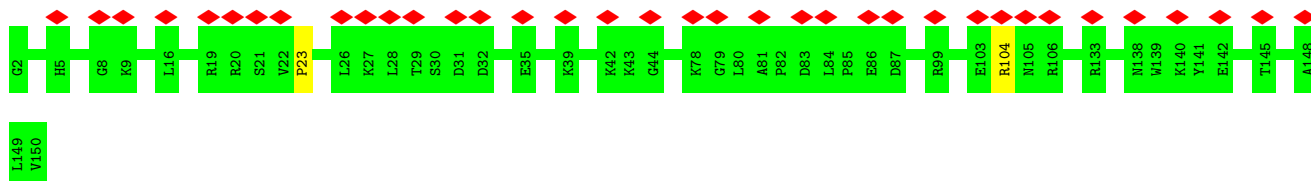
• Molecule 61: 40S ribosomal protein S11



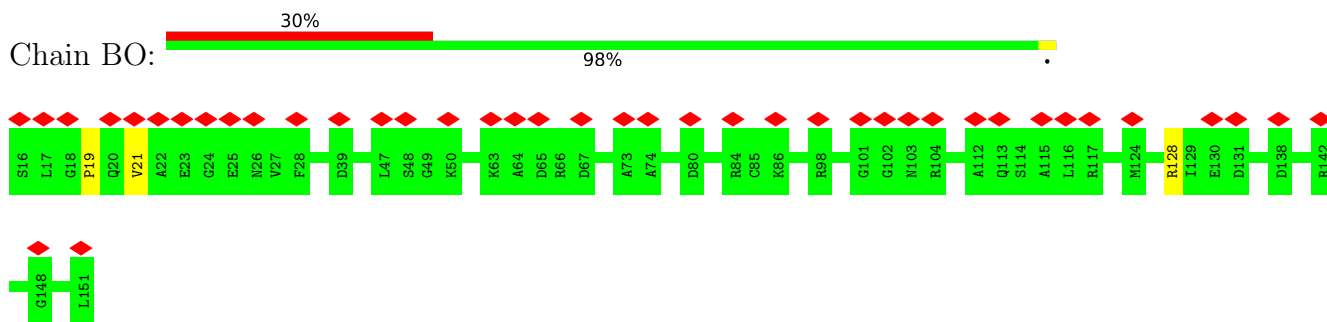
• Molecule 62: 40S ribosomal protein S12



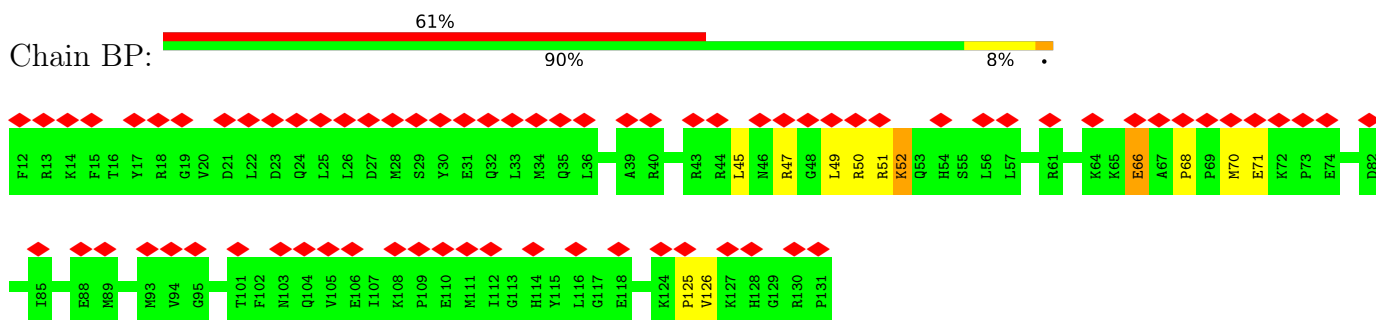
• Molecule 63: 40S ribosomal protein S13



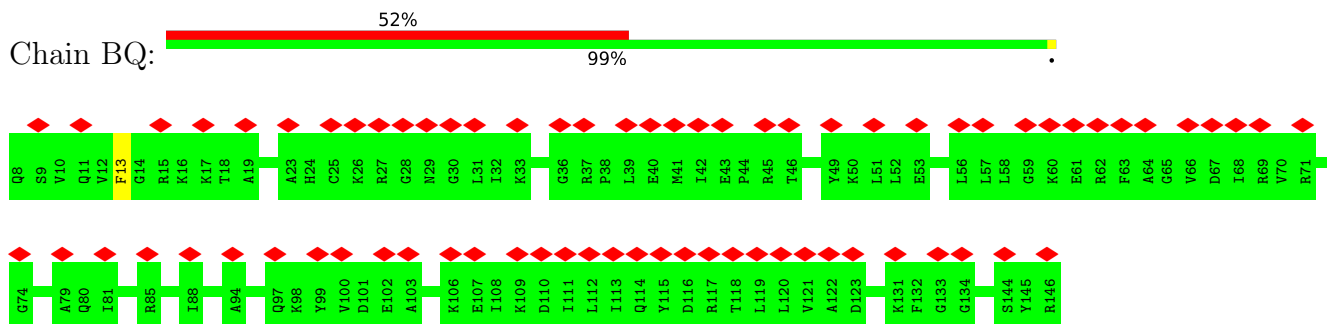
- Molecule 64: 40S ribosomal protein S14



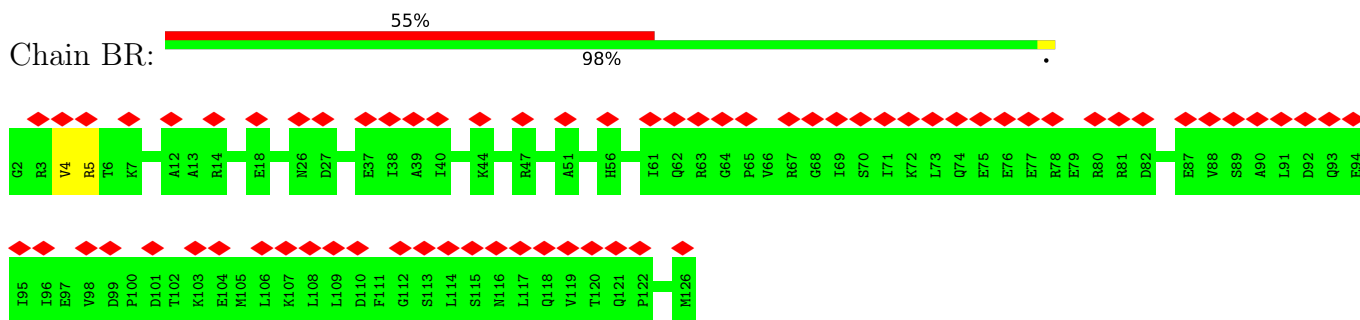
- Molecule 65: 40S ribosomal protein S15



- Molecule 66: 40S ribosomal protein S16

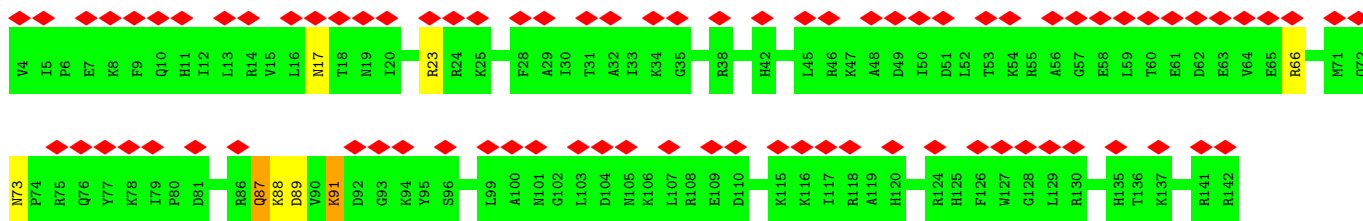


- Molecule 67: 40S ribosomal protein S17



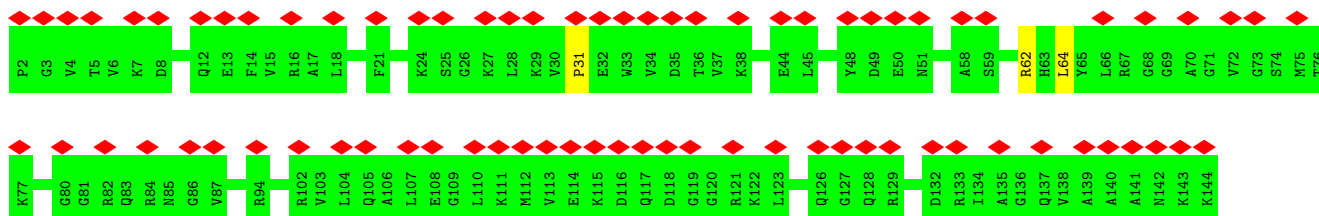
- Molecule 68: 40S ribosomal protein S18





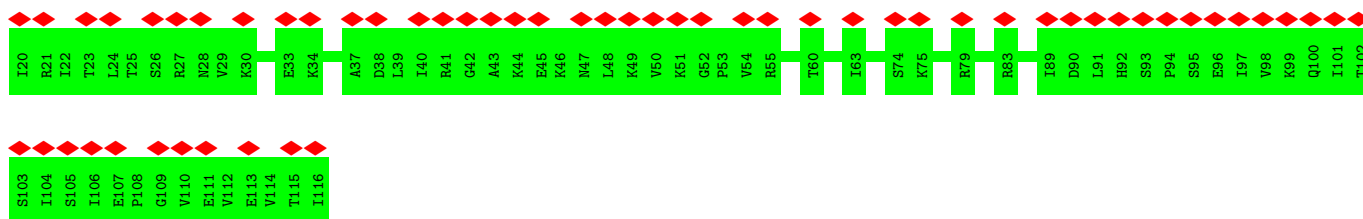
- Molecule 69: 40S ribosomal protein S19

Chain BT: 53% 98%



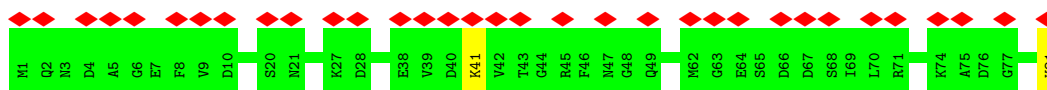
- Molecule 70: 40S ribosomal protein S20

Chain BU: 59% 100%



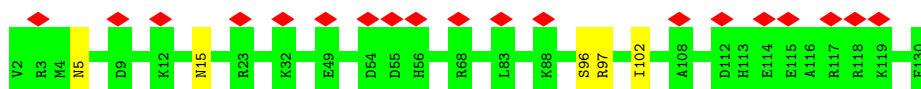
- Molecule 71: 40S ribosomal protein S21

Chain BV: 41% 98%



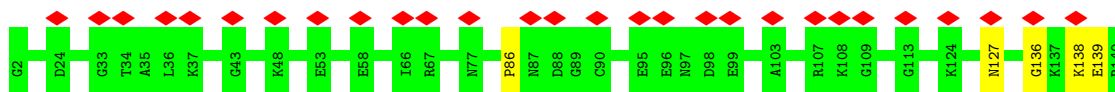
- Molecule 72: 40S ribosomal protein S15a

Chain BW: 15% 96%

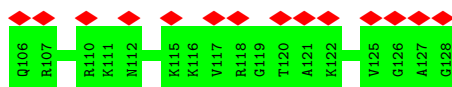
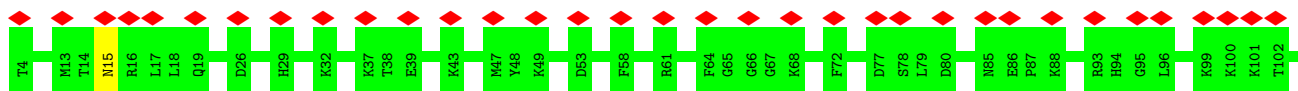
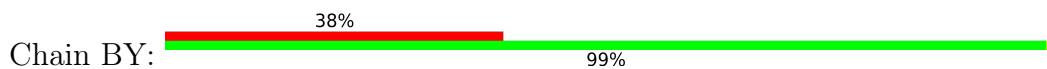


- Molecule 73: 40S ribosomal protein S23

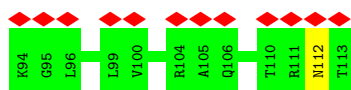
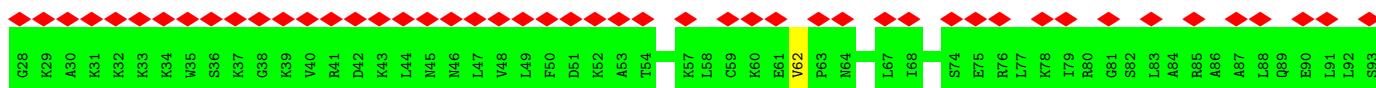
Chain BX: 20% 96%



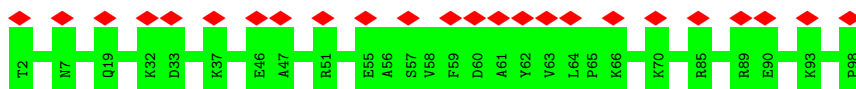
- Molecule 74: 40S ribosomal protein S24



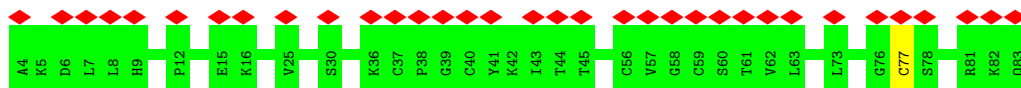
- Molecule 75: 40S ribosomal protein S25



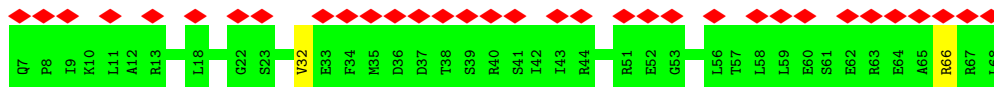
- Molecule 76: 40S ribosomal protein S26



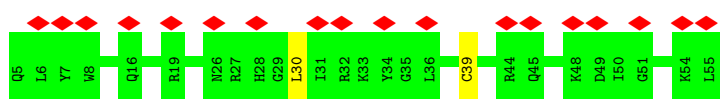
- Molecule 77: 40S ribosomal protein S27



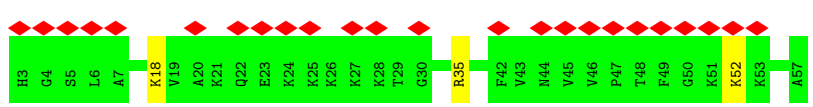
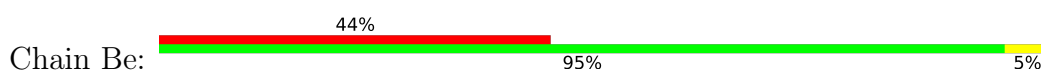
- Molecule 78: 40S ribosomal protein S28



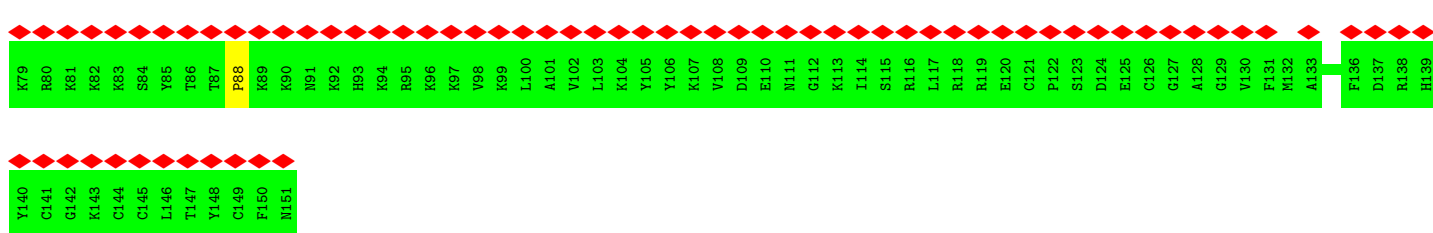
- Molecule 79: 40S ribosomal protein S29



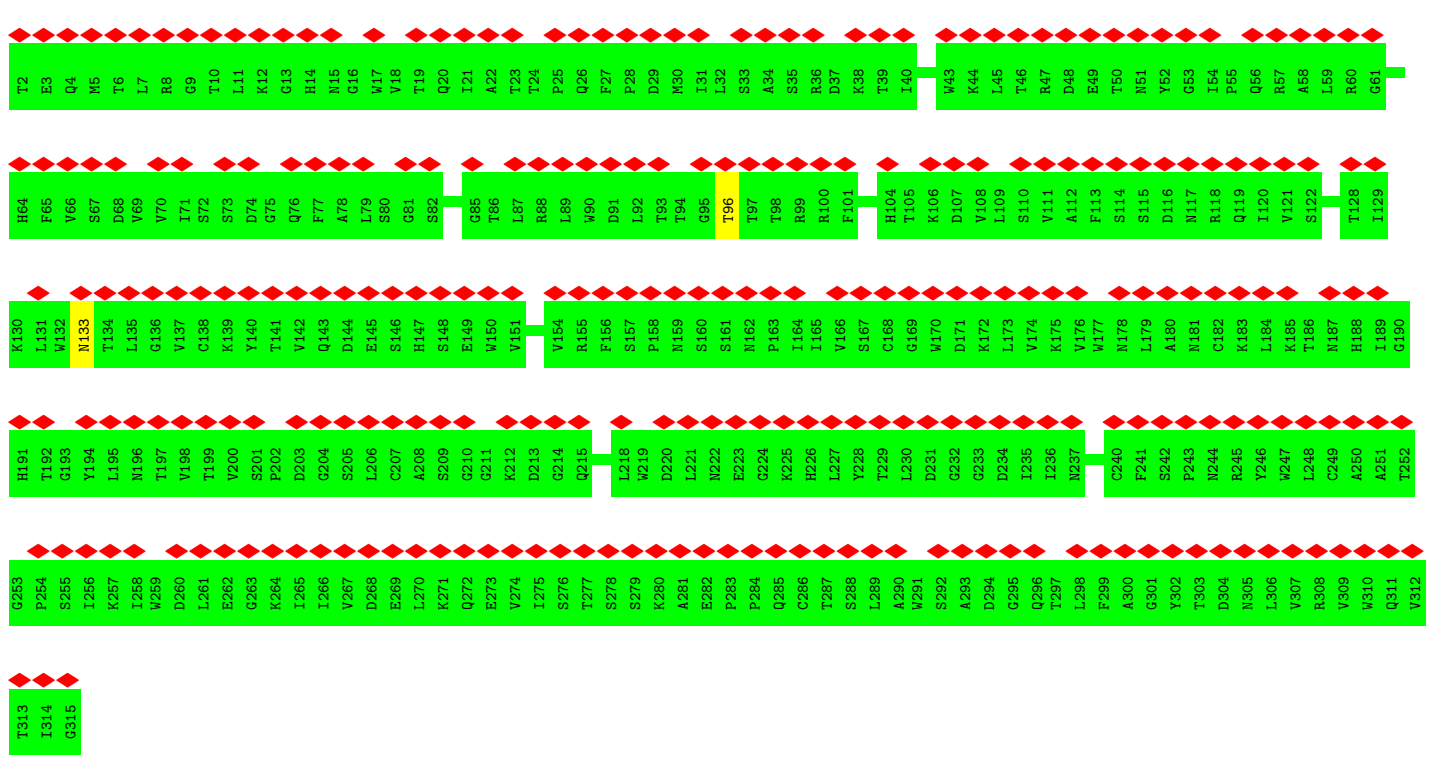
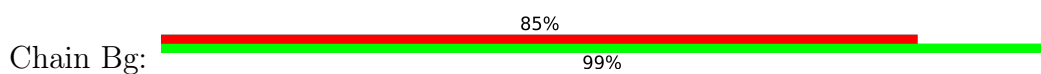
• Molecule 80: 40S ribosomal protein S30



• Molecule 81: 40S ribosomal protein S27a

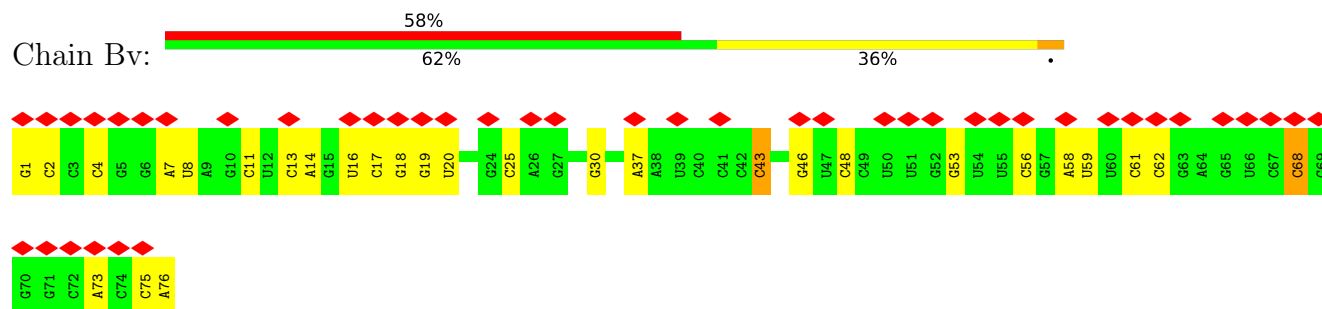


• Molecule 82: Receptor of activated protein C kinase 1

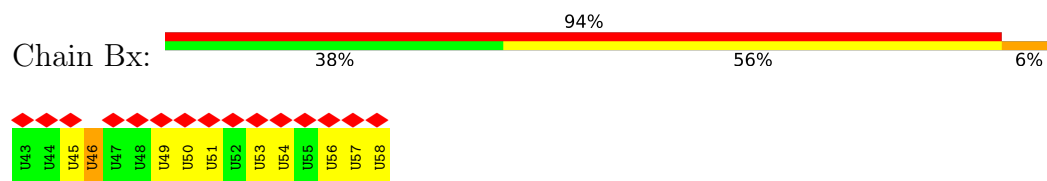




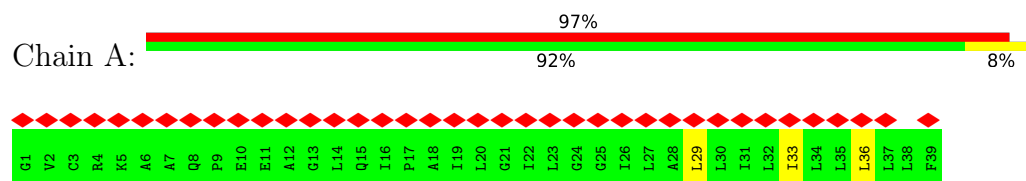
- Molecule 83: tRNA



- Molecule 84: mRNA



- Molecule 85: Cadherin-1



## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, Not provided       |           |
| Number of particles used             | 16594                     | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF         | Depositor |
| CTF correction method                | NONE                      | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                        | Depositor |
| Minimum defocus (nm)                 | Not provided              |           |
| Maximum defocus (nm)                 | Not provided              |           |
| Magnification                        | Not provided              |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value                    | 0.107                     | Depositor |
| Minimum map value                    | -0.054                    | Depositor |
| Average map value                    | 0.000                     | Depositor |
| Map value standard deviation         | 0.006                     | Depositor |
| Recommended contour level            | 0.02                      | Depositor |
| Map size ( $\text{\AA}$ )            | 471.5, 471.5, 471.5       | wwPDB     |
| Map dimensions                       | 410, 410, 410             | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.15, 1.15, 1.15          | Depositor |

## 5 Model quality i

### 5.1 Standard geometry i

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

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   | AA    | 0.40         | 0/1968      | 0.58        | 0/2639         |
| 2   | BA    | 0.36         | 0/1741      | 0.59        | 1/2366 (0.0%)  |
| 3   | AB    | 0.41         | 0/3246      | 0.61        | 1/4345 (0.0%)  |
| 4   | BB    | 0.34         | 0/1749      | 0.61        | 0/2340         |
| 5   | AC    | 0.38         | 0/2942      | 0.60        | 0/3951         |
| 6   | BC    | 0.37         | 0/1761      | 0.59        | 0/2379         |
| 7   | A3    | 0.66         | 0/3726      | 1.15        | 19/5804 (0.3%) |
| 8   | A4    | 0.66         | 0/2839      | 1.16        | 16/4425 (0.4%) |
| 9   | AD    | 0.37         | 0/2437      | 0.55        | 0/3262         |
| 10  | AE    | 0.35         | 0/1603      | 0.61        | 0/2153         |
| 11  | AF    | 0.39         | 0/1986      | 0.59        | 1/2644 (0.0%)  |
| 12  | AG    | 0.36         | 0/1913      | 0.60        | 1/2576 (0.0%)  |
| 13  | AH    | 0.36         | 0/1545      | 0.61        | 1/2077 (0.0%)  |
| 14  | AI    | 0.38         | 0/1730      | 0.56        | 0/2311         |
| 15  | AJ    | 0.35         | 0/1376      | 0.57        | 0/1841         |
| 16  | AK    | 0.33         | 0/886       | 0.79        | 2/1188 (0.2%)  |
| 17  | AL    | 0.37         | 0/1688      | 0.63        | 0/2260         |
| 18  | AM    | 0.42         | 0/1161      | 0.58        | 0/1554         |
| 19  | AN    | 0.46         | 0/1746      | 0.58        | 0/2338         |
| 20  | AO    | 0.41         | 0/1638      | 0.60        | 0/2191         |
| 21  | AP    | 0.40         | 0/1268      | 0.53        | 0/1701         |
| 22  | AQ    | 0.39         | 0/1537      | 0.68        | 1/2052 (0.0%)  |
| 23  | AR    | 0.35         | 0/1533      | 0.59        | 0/2025         |
| 24  | AS    | 0.42         | 0/1488      | 0.58        | 0/1997         |
| 25  | AT    | 0.42         | 0/1312      | 0.54        | 0/1753         |
| 26  | AU    | 0.37         | 0/822       | 0.51        | 0/1103         |
| 27  | AV    | 0.39         | 0/983       | 0.55        | 0/1319         |
| 28  | AW    | 0.36         | 0/1004      | 0.60        | 2/1332 (0.2%)  |
| 29  | AX    | 0.35         | 0/975       | 0.55        | 0/1312         |
| 30  | AY    | 0.37         | 0/1081      | 0.54        | 0/1439         |
| 31  | AZ    | 0.37         | 0/1126      | 0.59        | 0/1502         |
| 32  | Aa    | 0.42         | 0/1191      | 0.60        | 0/1591         |

| Mol | Chain | Bond lengths |                | Bond angles |                   |
|-----|-------|--------------|----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5           |
| 33  | Ab    | 0.33         | 0/569          | 0.62        | 1/750 (0.1%)      |
| 34  | Ac    | 0.36         | 0/812          | 0.58        | 1/1089 (0.1%)     |
| 35  | Ad    | 0.37         | 0/894          | 0.59        | 0/1204            |
| 36  | Ae    | 0.37         | 0/1082         | 0.59        | 0/1443            |
| 37  | Af    | 0.44         | 0/895          | 0.64        | 1/1198 (0.1%)     |
| 38  | Ag    | 0.39         | 0/916          | 0.63        | 0/1220            |
| 39  | Ah    | 0.33         | 0/1023         | 0.59        | 2/1351 (0.1%)     |
| 40  | Ai    | 0.34         | 0/805          | 0.57        | 0/1065            |
| 41  | Aj    | 0.41         | 0/703          | 0.65        | 0/929             |
| 42  | Ak    | 0.32         | 0/575          | 0.66        | 1/761 (0.1%)      |
| 43  | Al    | 0.36         | 0/454          | 0.56        | 0/599             |
| 44  | Am    | 0.35         | 0/417          | 0.61        | 0/553             |
| 45  | An    | 0.37         | 0/241          | 0.60        | 0/305             |
| 46  | Ao    | 0.38         | 0/877          | 0.59        | 0/1156            |
| 47  | Ap    | 0.43         | 0/718          | 0.60        | 0/953             |
| 48  | Aq    | 0.29         | 0/1058         | 0.75        | 1/1424 (0.1%)     |
| 49  | At    | 0.37         | 0/995          | 0.72        | 1/1334 (0.1%)     |
| 50  | Au    | 0.28         | 0/1772         | 0.59        | 1/2375 (0.0%)     |
| 51  | A2    | 0.68         | 1/86613 (0.0%) | 1.19        | 613/135108 (0.5%) |
| 52  | B1    | 0.57         | 1/40767 (0.0%) | 1.18        | 333/63536 (0.5%)  |
| 53  | BD    | 0.33         | 0/1736         | 0.54        | 0/2338            |
| 54  | BE    | 0.34         | 0/2072         | 0.59        | 0/2793            |
| 55  | BF    | 0.32         | 0/1524         | 0.60        | 0/2048            |
| 56  | BG    | 0.31         | 0/1907         | 0.59        | 0/2538            |
| 57  | BH    | 0.32         | 0/1501         | 0.57        | 0/2009            |
| 58  | BI    | 0.36         | 0/1725         | 0.59        | 0/2298            |
| 59  | BJ    | 0.32         | 0/1520         | 0.60        | 1/2030 (0.0%)     |
| 60  | BK    | 0.35         | 0/851          | 0.71        | 1/1147 (0.1%)     |
| 61  | BL    | 0.36         | 0/1281         | 0.63        | 1/1710 (0.1%)     |
| 62  | BM    | 0.28         | 0/941          | 0.60        | 0/1264            |
| 63  | BN    | 0.35         | 0/1226         | 0.60        | 0/1649            |
| 64  | BO    | 0.33         | 0/1029         | 0.58        | 0/1380            |
| 65  | BP    | 0.31         | 0/1019         | 0.64        | 0/1361            |
| 66  | BQ    | 0.32         | 0/1126         | 0.61        | 0/1506            |
| 67  | BR    | 0.31         | 0/1023         | 0.61        | 0/1373            |
| 68  | BS    | 0.29         | 0/1172         | 0.53        | 0/1570            |
| 69  | BT    | 0.34         | 0/1131         | 0.61        | 1/1515 (0.1%)     |
| 70  | BU    | 0.30         | 0/778          | 0.56        | 0/1045            |
| 71  | BV    | 0.33         | 0/623          | 0.57        | 0/833             |
| 72  | BW    | 0.36         | 0/1051         | 0.58        | 0/1406            |
| 73  | BX    | 0.37         | 0/1097         | 0.60        | 0/1464            |
| 74  | BY    | 0.34         | 0/1032         | 0.61        | 0/1371            |
| 75  | BZ    | 0.32         | 0/696          | 0.66        | 0/929             |

| Mol | Chain | Bond lengths |                 | Bond angles |                    |
|-----|-------|--------------|-----------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5            |
| 76  | Ba    | 0.37         | 0/786           | 0.61        | 0/1053             |
| 77  | Bb    | 0.32         | 0/637           | 0.55        | 0/854              |
| 78  | Bc    | 0.29         | 0/490           | 0.56        | 0/656              |
| 79  | Bd    | 0.38         | 0/437           | 0.70        | 2/580 (0.3%)       |
| 80  | Be    | 0.32         | 0/443           | 0.61        | 0/583              |
| 81  | Bf    | 0.29         | 0/613           | 0.58        | 0/811              |
| 82  | Bg    | 0.31         | 0/2497          | 0.58        | 0/3399             |
| 83  | Bv    | 0.59         | 2/1813 (0.1%)   | 1.21        | 18/2823 (0.6%)     |
| 84  | Bx    | 0.28         | 0/351           | 1.07        | 3/540 (0.6%)       |
| 85  | A     | 0.29         | 0/189           | 0.64        | 0/260              |
| All | All   | 0.55         | 4/232504 (0.0%) | 1.00        | 1027/341259 (0.3%) |

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 |
|-----|-------|---------------------|---------------------|
| 4   | BB    | 0                   | 1                   |
| 9   | AD    | 0                   | 1                   |
| 13  | AH    | 0                   | 1                   |
| 29  | AX    | 0                   | 1                   |
| All | All   | 0                   | 4                   |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 83  | Bv    | 73  | A    | O3'-P | 14.03  | 1.77        | 1.61     |
| 52  | B1    | 1   | U    | OP3-P | -10.73 | 1.48        | 1.61     |
| 83  | Bv    | 1   | G    | OP3-P | -10.71 | 1.48        | 1.61     |
| 51  | A2    | 930 | A    | N9-C4 | -5.15  | 1.34        | 1.37     |

All (1027) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 52  | B1    | 1288 | U    | C2-N1-C1' | 10.38 | 130.16      | 117.70   |
| 51  | A2    | 463  | C    | N1-C2-O2  | 10.12 | 124.97      | 118.90   |
| 52  | B1    | 1398 | G    | C4-N9-C1' | 10.06 | 139.57      | 126.50   |
| 52  | B1    | 984  | C    | N3-C2-O2  | -9.83 | 115.02      | 121.90   |
| 52  | B1    | 1464 | C    | N1-C2-O2  | 9.81  | 124.79      | 118.90   |
| 51  | A2    | 2388 | U    | C2-N1-C1' | 9.79  | 129.45      | 117.70   |
| 51  | A2    | 480  | C    | N1-C2-O2  | 9.71  | 124.73      | 118.90   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 52  | B1    | 118  | C    | N1-C2-O2  | 9.64  | 124.68      | 118.90   |
| 51  | A2    | 2447 | U    | N3-C2-O2  | -9.61 | 115.47      | 122.20   |
| 52  | B1    | 67   | C    | N1-C2-O2  | 9.54  | 124.63      | 118.90   |
| 8   | A4    | 29   | C    | N1-C2-O2  | 9.47  | 124.58      | 118.90   |
| 52  | B1    | 621  | C    | N1-C2-O2  | 9.43  | 124.56      | 118.90   |
| 52  | B1    | 1271 | C    | N1-C2-O2  | 9.30  | 124.48      | 118.90   |
| 51  | A2    | 219  | C    | C2-N1-C1' | 9.27  | 129.00      | 118.80   |
| 52  | B1    | 96   | C    | C2-N1-C1' | 9.20  | 128.92      | 118.80   |
| 51  | A2    | 1576 | C    | C2-N1-C1' | 9.20  | 128.92      | 118.80   |
| 51  | A2    | 2398 | C    | C2-N1-C1' | 9.11  | 128.82      | 118.80   |
| 7   | A3    | 126  | C    | C2-N1-C1' | 9.10  | 128.81      | 118.80   |
| 52  | B1    | 89   | C    | C2-N1-C1' | 9.08  | 128.78      | 118.80   |
| 52  | B1    | 1464 | C    | C2-N1-C1' | 9.03  | 128.73      | 118.80   |
| 51  | A2    | 1256 | G    | C2-N3-C4  | 8.97  | 116.39      | 111.90   |
| 51  | A2    | 4887 | C    | N1-C2-O2  | 8.95  | 124.27      | 118.90   |
| 52  | B1    | 118  | C    | C2-N1-C1' | 8.95  | 128.65      | 118.80   |
| 7   | A3    | 126  | C    | N1-C2-O2  | 8.88  | 124.23      | 118.90   |
| 52  | B1    | 67   | C    | C2-N1-C1' | 8.88  | 128.56      | 118.80   |
| 52  | B1    | 568  | C    | N1-C2-O2  | 8.82  | 124.19      | 118.90   |
| 51  | A2    | 4886 | C    | N1-C2-O2  | 8.81  | 124.19      | 118.90   |
| 52  | B1    | 621  | C    | C2-N1-C1' | 8.80  | 128.48      | 118.80   |
| 52  | B1    | 1398 | G    | C8-N9-C1' | -8.79 | 115.57      | 127.00   |
| 51  | A2    | 1256 | G    | N3-C4-C5  | -8.76 | 124.22      | 128.60   |
| 52  | B1    | 621  | C    | N3-C2-O2  | -8.72 | 115.80      | 121.90   |
| 83  | Bv    | 20   | U    | N1-C2-O2  | 8.70  | 128.89      | 122.80   |
| 52  | B1    | 96   | C    | N1-C2-O2  | 8.66  | 124.10      | 118.90   |
| 52  | B1    | 742  | U    | N3-C2-O2  | -8.64 | 116.15      | 122.20   |
| 52  | B1    | 742  | U    | N1-C2-O2  | 8.64  | 128.85      | 122.80   |
| 51  | A2    | 480  | C    | N3-C2-O2  | -8.62 | 115.86      | 121.90   |
| 51  | A2    | 1259 | C    | C6-N1-C2  | -8.62 | 116.85      | 120.30   |
| 51  | A2    | 645  | C    | C2-N1-C1' | 8.56  | 128.22      | 118.80   |
| 51  | A2    | 256  | C    | N1-C2-O2  | 8.54  | 124.03      | 118.90   |
| 51  | A2    | 4010 | C    | N1-C2-O2  | 8.53  | 124.02      | 118.90   |
| 51  | A2    | 918  | C    | N1-C2-O2  | 8.51  | 124.00      | 118.90   |
| 51  | A2    | 163  | C    | N1-C2-O2  | 8.49  | 123.99      | 118.90   |
| 51  | A2    | 1576 | C    | N3-C2-O2  | -8.48 | 115.96      | 121.90   |
| 51  | A2    | 256  | C    | N3-C2-O2  | -8.48 | 115.97      | 121.90   |
| 52  | B1    | 1811 | C    | C2-N1-C1' | 8.47  | 128.12      | 118.80   |
| 51  | A2    | 2282 | C    | N1-C2-O2  | 8.44  | 123.97      | 118.90   |
| 83  | Bv    | 20   | U    | C2-N1-C1' | 8.40  | 127.78      | 117.70   |
| 51  | A2    | 2398 | C    | N1-C2-O2  | 8.40  | 123.94      | 118.90   |
| 51  | A2    | 1564 | U    | C2-N1-C1' | 8.39  | 127.77      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 51  | A2    | 463  | C    | N3-C2-O2  | -8.38 | 116.04      | 121.90   |
| 52  | B1    | 96   | C    | N3-C2-O2  | -8.38 | 116.04      | 121.90   |
| 51  | A2    | 1067 | C    | N1-C2-O2  | 8.36  | 123.92      | 118.90   |
| 51  | A2    | 2389 | C    | C2-N1-C1' | 8.36  | 128.00      | 118.80   |
| 51  | A2    | 480  | C    | C6-N1-C2  | -8.36 | 116.96      | 120.30   |
| 52  | B1    | 1288 | U    | N1-C2-O2  | 8.36  | 128.65      | 122.80   |
| 52  | B1    | 1551 | U    | C2-N1-C1' | 8.32  | 127.69      | 117.70   |
| 51  | A2    | 1576 | C    | N1-C2-O2  | 8.29  | 123.88      | 118.90   |
| 3   | AB    | 292  | LEU  | CA-CB-CG  | 8.27  | 134.31      | 115.30   |
| 8   | A4    | 14   | C    | C2-N1-C1' | 8.25  | 127.88      | 118.80   |
| 51  | A2    | 4088 | C    | N1-C2-O2  | 8.22  | 123.83      | 118.90   |
| 52  | B1    | 1520 | G    | N3-C4-C5  | -8.21 | 124.49      | 128.60   |
| 51  | A2    | 2447 | U    | C6-N1-C2  | -8.21 | 116.08      | 121.00   |
| 51  | A2    | 1499 | G    | C4-N9-C1' | 8.20  | 137.17      | 126.50   |
| 52  | B1    | 1315 | U    | C2-N1-C1' | 8.20  | 127.54      | 117.70   |
| 51  | A2    | 514  | C    | N3-C2-O2  | -8.19 | 116.17      | 121.90   |
| 51  | A2    | 2282 | C    | N3-C2-O2  | -8.18 | 116.17      | 121.90   |
| 8   | A4    | 29   | C    | N3-C2-O2  | -8.15 | 116.20      | 121.90   |
| 51  | A2    | 674  | C    | N1-C2-O2  | 8.11  | 123.77      | 118.90   |
| 51  | A2    | 2330 | C    | C2-N1-C1' | 8.09  | 127.70      | 118.80   |
| 51  | A2    | 4884 | C    | C6-N1-C2  | -8.08 | 117.07      | 120.30   |
| 83  | Bv    | 43   | C    | N1-C2-O2  | 8.04  | 123.72      | 118.90   |
| 51  | A2    | 77   | U    | N3-C2-O2  | -8.03 | 116.58      | 122.20   |
| 52  | B1    | 1315 | U    | N1-C2-O2  | 8.03  | 128.42      | 122.80   |
| 52  | B1    | 1520 | G    | C4-N9-C1' | 8.02  | 136.93      | 126.50   |
| 51  | A2    | 514  | C    | N1-C2-O2  | 8.01  | 123.70      | 118.90   |
| 51  | A2    | 3607 | C    | N3-C2-O2  | -8.00 | 116.30      | 121.90   |
| 51  | A2    | 4602 | C    | N1-C2-O2  | 8.00  | 123.70      | 118.90   |
| 51  | A2    | 180  | C    | N1-C2-O2  | 7.97  | 123.68      | 118.90   |
| 51  | A2    | 480  | C    | C2-N1-C1' | 7.95  | 127.55      | 118.80   |
| 51  | A2    | 1938 | U    | N3-C2-O2  | -7.92 | 116.65      | 122.20   |
| 51  | A2    | 649  | C    | N1-C2-O2  | 7.91  | 123.65      | 118.90   |
| 51  | A2    | 4880 | C    | C2-N1-C1' | 7.91  | 127.50      | 118.80   |
| 51  | A2    | 4602 | C    | C2-N1-C1' | 7.89  | 127.48      | 118.80   |
| 52  | B1    | 879  | C    | N1-C2-O2  | 7.88  | 123.63      | 118.90   |
| 51  | A2    | 1989 | U    | N1-C2-O2  | 7.87  | 128.31      | 122.80   |
| 51  | A2    | 4276 | C    | N1-C2-O2  | 7.86  | 123.62      | 118.90   |
| 52  | B1    | 1389 | C    | C2-N1-C1' | 7.83  | 127.42      | 118.80   |
| 52  | B1    | 1019 | C    | N3-C2-O2  | -7.83 | 116.42      | 121.90   |
| 51  | A2    | 4671 | U    | N3-C2-O2  | -7.82 | 116.73      | 122.20   |
| 51  | A2    | 197  | U    | N3-C2-O2  | -7.81 | 116.73      | 122.20   |
| 52  | B1    | 918  | U    | N1-C2-O2  | 7.78  | 128.25      | 122.80   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 51  | A2    | 2388 | U    | N1-C2-O2  | 7.77  | 128.24      | 122.80   |
| 51  | A2    | 197  | U    | C2-N1-C1' | 7.77  | 127.02      | 117.70   |
| 51  | A2    | 219  | C    | N1-C2-O2  | 7.76  | 123.56      | 118.90   |
| 52  | B1    | 984  | C    | N1-C2-O2  | 7.76  | 123.56      | 118.90   |
| 52  | B1    | 1624 | U    | N1-C2-O2  | 7.76  | 128.23      | 122.80   |
| 51  | A2    | 2388 | U    | N3-C2-O2  | -7.75 | 116.78      | 122.20   |
| 51  | A2    | 4887 | C    | N3-C2-O2  | -7.73 | 116.49      | 121.90   |
| 51  | A2    | 2447 | U    | N1-C2-O2  | 7.73  | 128.21      | 122.80   |
| 51  | A2    | 2751 | C    | C6-N1-C2  | -7.72 | 117.21      | 120.30   |
| 51  | A2    | 2799 | C    | N1-C2-O2  | 7.71  | 123.53      | 118.90   |
| 52  | B1    | 210  | U    | N1-C2-O2  | 7.71  | 128.20      | 122.80   |
| 51  | A2    | 4671 | U    | N1-C2-O2  | 7.68  | 128.18      | 122.80   |
| 51  | A2    | 1938 | U    | N1-C2-O2  | 7.68  | 128.18      | 122.80   |
| 51  | A2    | 1989 | U    | N3-C2-O2  | -7.68 | 116.83      | 122.20   |
| 51  | A2    | 219  | C    | C6-N1-C2  | -7.67 | 117.23      | 120.30   |
| 8   | A4    | 14   | C    | N1-C2-O2  | 7.66  | 123.50      | 118.90   |
| 51  | A2    | 2727 | C    | C2-N1-C1' | 7.64  | 127.21      | 118.80   |
| 51  | A2    | 3890 | C    | C2-N1-C1' | 7.64  | 127.20      | 118.80   |
| 52  | B1    | 1464 | C    | N3-C2-O2  | -7.63 | 116.56      | 121.90   |
| 52  | B1    | 1551 | U    | N1-C2-O2  | 7.62  | 128.14      | 122.80   |
| 51  | A2    | 905  | G    | C8-N9-C4  | -7.62 | 103.35      | 106.40   |
| 51  | A2    | 674  | C    | N3-C2-O2  | -7.61 | 116.57      | 121.90   |
| 51  | A2    | 1266 | G    | C8-N9-C4  | -7.60 | 103.36      | 106.40   |
| 52  | B1    | 1271 | C    | N3-C2-O2  | -7.60 | 116.58      | 121.90   |
| 51  | A2    | 345  | C    | N3-C2-O2  | -7.59 | 116.59      | 121.90   |
| 51  | A2    | 927  | C    | C2-N1-C1' | 7.59  | 127.15      | 118.80   |
| 52  | B1    | 950  | C    | C2-N1-C1' | 7.59  | 127.15      | 118.80   |
| 51  | A2    | 3664 | U    | N3-C2-O2  | -7.59 | 116.89      | 122.20   |
| 52  | B1    | 1315 | U    | N3-C2-O2  | -7.58 | 116.89      | 122.20   |
| 52  | B1    | 853  | C    | N1-C2-O2  | 7.58  | 123.45      | 118.90   |
| 51  | A2    | 4011 | C    | N1-C2-O2  | 7.57  | 123.44      | 118.90   |
| 51  | A2    | 4088 | C    | C2-N1-C1' | 7.56  | 127.11      | 118.80   |
| 51  | A2    | 1596 | C    | N1-C2-O2  | 7.55  | 123.43      | 118.90   |
| 51  | A2    | 4169 | C    | C2-N1-C1' | 7.54  | 127.09      | 118.80   |
| 51  | A2    | 1959 | C    | N1-C2-O2  | 7.53  | 123.42      | 118.90   |
| 51  | A2    | 2325 | C    | N1-C2-O2  | 7.52  | 123.41      | 118.90   |
| 51  | A2    | 1466 | G    | N3-C4-C5  | -7.51 | 124.85      | 128.60   |
| 8   | A4    | 29   | C    | C2-N1-C1' | 7.50  | 127.05      | 118.80   |
| 51  | A2    | 703  | C    | N1-C2-O2  | 7.49  | 123.40      | 118.90   |
| 51  | A2    | 1284 | C    | C6-N1-C2  | -7.49 | 117.31      | 120.30   |
| 51  | A2    | 2499 | C    | C2-N1-C1' | 7.49  | 127.03      | 118.80   |
| 83  | Bv    | 20   | U    | N3-C2-O2  | -7.48 | 116.97      | 122.20   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 51  | A2    | 1350 | C    | N1-C2-O2  | 7.46  | 123.38      | 118.90   |
| 52  | B1    | 53   | C    | C6-N1-C2  | -7.46 | 117.32      | 120.30   |
| 52  | B1    | 1288 | U    | N3-C2-O2  | -7.45 | 116.98      | 122.20   |
| 51  | A2    | 2447 | U    | C5-C6-N1  | 7.43  | 126.42      | 122.70   |
| 52  | B1    | 1261 | C    | C6-N1-C2  | -7.43 | 117.33      | 120.30   |
| 52  | B1    | 1557 | C    | N1-C2-O2  | 7.41  | 123.34      | 118.90   |
| 52  | B1    | 119  | U    | N3-C2-O2  | -7.41 | 117.02      | 122.20   |
| 51  | A2    | 197  | U    | N1-C2-O2  | 7.40  | 127.98      | 122.80   |
| 51  | A2    | 1193 | C    | N1-C2-O2  | 7.37  | 123.32      | 118.90   |
| 51  | A2    | 2478 | C    | N3-C2-O2  | -7.37 | 116.74      | 121.90   |
| 51  | A2    | 3725 | G    | N3-C4-N9  | -7.37 | 121.58      | 126.00   |
| 51  | A2    | 1466 | G    | C4-N9-C1' | 7.36  | 136.06      | 126.50   |
| 52  | B1    | 1292 | C    | N1-C2-O2  | 7.36  | 123.31      | 118.90   |
| 52  | B1    | 227  | U    | P-O3'-C3' | 7.35  | 128.52      | 119.70   |
| 52  | B1    | 1586 | U    | C2-N1-C1' | 7.35  | 126.52      | 117.70   |
| 51  | A2    | 2398 | C    | N3-C2-O2  | -7.34 | 116.76      | 121.90   |
| 51  | A2    | 1653 | U    | N3-C2-O2  | -7.33 | 117.07      | 122.20   |
| 51  | A2    | 251  | G    | C4-N9-C1' | 7.31  | 136.00      | 126.50   |
| 51  | A2    | 4729 | C    | N1-C2-O2  | 7.31  | 123.29      | 118.90   |
| 52  | B1    | 118  | C    | N3-C2-O2  | -7.30 | 116.79      | 121.90   |
| 7   | A3    | 96   | C    | N1-C2-O2  | 7.29  | 123.28      | 118.90   |
| 51  | A2    | 645  | C    | C6-N1-C2  | -7.27 | 117.39      | 120.30   |
| 51  | A2    | 940  | C    | N3-C2-O2  | -7.27 | 116.81      | 121.90   |
| 51  | A2    | 2499 | C    | N1-C2-O2  | 7.26  | 123.26      | 118.90   |
| 52  | B1    | 89   | C    | N1-C2-O2  | 7.26  | 123.26      | 118.90   |
| 52  | B1    | 1389 | C    | N3-C2-O2  | -7.25 | 116.82      | 121.90   |
| 51  | A2    | 1466 | G    | N3-C4-N9  | 7.25  | 130.35      | 126.00   |
| 51  | A2    | 1596 | C    | N3-C2-O2  | -7.25 | 116.82      | 121.90   |
| 51  | A2    | 2325 | C    | C2-N1-C1' | 7.25  | 126.77      | 118.80   |
| 51  | A2    | 233  | G    | N3-C2-N2  | -7.24 | 114.83      | 119.90   |
| 52  | B1    | 984  | C    | C6-N1-C2  | -7.22 | 117.41      | 120.30   |
| 51  | A2    | 905  | G    | C4-N9-C1' | 7.22  | 135.89      | 126.50   |
| 51  | A2    | 463  | C    | C2-N1-C1' | 7.20  | 126.72      | 118.80   |
| 83  | Bv    | 43   | C    | C6-N1-C2  | -7.20 | 117.42      | 120.30   |
| 52  | B1    | 1123 | C    | C2-N1-C1' | 7.19  | 126.71      | 118.80   |
| 51  | A2    | 2032 | C    | C6-N1-C2  | -7.19 | 117.42      | 120.30   |
| 52  | B1    | 1624 | U    | C2-N1-C1' | 7.18  | 126.32      | 117.70   |
| 51  | A2    | 2400 | G    | C4-N9-C1' | 7.18  | 135.83      | 126.50   |
| 51  | A2    | 3607 | C    | N1-C2-O2  | 7.17  | 123.20      | 118.90   |
| 51  | A2    | 4887 | C    | C2-N1-C1' | 7.17  | 126.69      | 118.80   |
| 51  | A2    | 671  | C    | N1-C2-O2  | 7.17  | 123.20      | 118.90   |
| 52  | B1    | 1271 | C    | C2-N1-C1' | 7.16  | 126.68      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 52  | B1    | 1756 | C    | P-O3'-C3' | 7.16  | 128.29      | 119.70   |
| 51  | A2    | 3880 | C    | N1-C2-O2  | 7.15  | 123.19      | 118.90   |
| 51  | A2    | 4276 | C    | N3-C2-O2  | -7.14 | 116.90      | 121.90   |
| 52  | B1    | 1557 | C    | C2-N1-C1' | 7.14  | 126.65      | 118.80   |
| 52  | B1    | 1389 | C    | C6-N1-C2  | -7.14 | 117.45      | 120.30   |
| 51  | A2    | 119  | G    | C4-N9-C1' | 7.13  | 135.77      | 126.50   |
| 52  | B1    | 1586 | U    | N1-C2-O2  | 7.13  | 127.79      | 122.80   |
| 51  | A2    | 3664 | U    | N1-C2-O2  | 7.13  | 127.79      | 122.80   |
| 51  | A2    | 4884 | C    | N1-C2-O2  | 7.13  | 123.18      | 118.90   |
| 51  | A2    | 905  | G    | N3-C4-C5  | -7.12 | 125.04      | 128.60   |
| 51  | A2    | 3890 | C    | C6-N1-C2  | -7.12 | 117.45      | 120.30   |
| 51  | A2    | 3863 | U    | N3-C2-O2  | -7.12 | 117.22      | 122.20   |
| 59  | BJ    | 119  | LEU  | CA-CB-CG  | 7.10  | 131.64      | 115.30   |
| 52  | B1    | 174  | C    | C2-N1-C1' | 7.10  | 126.61      | 118.80   |
| 52  | B1    | 1389 | C    | N1-C2-O2  | 7.10  | 123.16      | 118.90   |
| 51  | A2    | 119  | G    | N3-C4-N9  | 7.09  | 130.26      | 126.00   |
| 52  | B1    | 1019 | C    | N1-C2-O2  | 7.09  | 123.16      | 118.90   |
| 52  | B1    | 119  | U    | N1-C2-O2  | 7.09  | 127.76      | 122.80   |
| 51  | A2    | 4010 | C    | N3-C2-O2  | -7.09 | 116.94      | 121.90   |
| 52  | B1    | 1512 | C    | C2-N1-C1' | 7.08  | 126.59      | 118.80   |
| 51  | A2    | 2478 | C    | N1-C2-O2  | 7.08  | 123.15      | 118.90   |
| 52  | B1    | 179  | C    | N1-C2-O2  | 7.08  | 123.14      | 118.90   |
| 51  | A2    | 2447 | U    | C2-N1-C1' | 7.07  | 126.19      | 117.70   |
| 51  | A2    | 4489 | G    | C4-N9-C1' | 7.06  | 135.68      | 126.50   |
| 51  | A2    | 493  | G    | C4-N9-C1' | 7.05  | 135.67      | 126.50   |
| 51  | A2    | 3759 | C    | N1-C2-O2  | 7.05  | 123.13      | 118.90   |
| 51  | A2    | 2606 | C    | N1-C2-O2  | 7.05  | 123.13      | 118.90   |
| 51  | A2    | 1564 | U    | N1-C2-O2  | 7.04  | 127.73      | 122.80   |
| 51  | A2    | 2373 | G    | C4-N9-C1' | 7.04  | 135.66      | 126.50   |
| 52  | B1    | 1315 | U    | C5-C6-N1  | 7.04  | 126.22      | 122.70   |
| 51  | A2    | 918  | C    | C2-N1-C1' | 7.01  | 126.51      | 118.80   |
| 83  | Bv    | 43   | C    | C2-N1-C1' | 7.01  | 126.51      | 118.80   |
| 51  | A2    | 163  | C    | N3-C2-O2  | -7.01 | 117.00      | 121.90   |
| 51  | A2    | 3880 | C    | C2-N1-C1' | 7.01  | 126.51      | 118.80   |
| 51  | A2    | 1428 | U    | N3-C2-O2  | -7.00 | 117.30      | 122.20   |
| 52  | B1    | 174  | C    | C6-N1-C2  | -6.99 | 117.50      | 120.30   |
| 7   | A3    | 129  | C    | N1-C2-O2  | 6.99  | 123.09      | 118.90   |
| 7   | A3    | 126  | C    | N3-C2-O2  | -6.98 | 117.02      | 121.90   |
| 52  | B1    | 1286 | G    | C4-N9-C1' | 6.97  | 135.57      | 126.50   |
| 52  | B1    | 1261 | C    | C2-N1-C1' | 6.97  | 126.47      | 118.80   |
| 51  | A2    | 1938 | U    | C2-N1-C1' | 6.96  | 126.06      | 117.70   |
| 52  | B1    | 1551 | U    | N3-C2-O2  | -6.96 | 117.33      | 122.20   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 51  | A2    | 4489 | G    | N3-C4-N9  | 6.96  | 130.17      | 126.00   |
| 51  | A2    | 1638 | U    | N3-C2-O2  | -6.94 | 117.34      | 122.20   |
| 52  | B1    | 1624 | U    | N3-C2-O2  | -6.93 | 117.35      | 122.20   |
| 51  | A2    | 647  | U    | N3-C2-O2  | -6.93 | 117.35      | 122.20   |
| 51  | A2    | 4671 | U    | C2-N1-C1' | 6.92  | 126.00      | 117.70   |
| 33  | Ab    | 54   | LEU  | CA-CB-CG  | 6.92  | 131.21      | 115.30   |
| 37  | Af    | 58   | VAL  | C-N-CA    | 6.92  | 138.99      | 121.70   |
| 52  | B1    | 402  | C    | N1-C2-O2  | 6.92  | 123.05      | 118.90   |
| 51  | A2    | 2000 | C    | N1-C2-O2  | 6.91  | 123.05      | 118.90   |
| 51  | A2    | 2398 | C    | C6-N1-C2  | -6.91 | 117.54      | 120.30   |
| 51  | A2    | 1067 | C    | N3-C2-O2  | -6.91 | 117.07      | 121.90   |
| 51  | A2    | 4462 | U    | N1-C2-O2  | 6.91  | 127.63      | 122.80   |
| 51  | A2    | 1966 | G    | C4-N9-C1' | 6.89  | 135.46      | 126.50   |
| 52  | B1    | 459  | C    | C2-N1-C1' | 6.89  | 126.38      | 118.80   |
| 51  | A2    | 3882 | C    | C6-N1-C2  | -6.88 | 117.55      | 120.30   |
| 52  | B1    | 1288 | U    | C6-N1-C1' | -6.88 | 111.56      | 121.20   |
| 51  | A2    | 1256 | G    | N3-C4-N9  | 6.88  | 130.13      | 126.00   |
| 52  | B1    | 1053 | C    | C2-N1-C1' | 6.88  | 126.36      | 118.80   |
| 52  | B1    | 1237 | C    | C2-N1-C1' | 6.87  | 126.36      | 118.80   |
| 51  | A2    | 647  | U    | N1-C2-O2  | 6.85  | 127.60      | 122.80   |
| 51  | A2    | 4886 | C    | C2-N1-C1' | 6.85  | 126.33      | 118.80   |
| 52  | B1    | 210  | U    | N3-C2-O2  | -6.85 | 117.41      | 122.20   |
| 52  | B1    | 1286 | G    | N3-C4-N9  | 6.84  | 130.11      | 126.00   |
| 51  | A2    | 1499 | G    | C8-N9-C1' | -6.84 | 118.11      | 127.00   |
| 52  | B1    | 797  | C    | C6-N1-C2  | -6.83 | 117.57      | 120.30   |
| 51  | A2    | 207  | C    | N1-C2-O2  | 6.83  | 123.00      | 118.90   |
| 52  | B1    | 1130 | G    | N3-C2-N2  | -6.83 | 115.12      | 119.90   |
| 51  | A2    | 441  | C    | C6-N1-C2  | -6.83 | 117.57      | 120.30   |
| 51  | A2    | 1746 | G    | N3-C4-N9  | 6.82  | 130.09      | 126.00   |
| 52  | B1    | 853  | C    | N3-C2-O2  | -6.82 | 117.13      | 121.90   |
| 51  | A2    | 345  | C    | N1-C2-O2  | 6.81  | 122.99      | 118.90   |
| 51  | A2    | 4103 | C    | C2-N1-C1' | 6.80  | 126.28      | 118.80   |
| 52  | B1    | 568  | C    | N3-C2-O2  | -6.79 | 117.14      | 121.90   |
| 2   | BA    | 201  | LEU  | CA-CB-CG  | 6.79  | 130.92      | 115.30   |
| 52  | B1    | 620  | G    | N3-C4-C5  | -6.79 | 125.20      | 128.60   |
| 51  | A2    | 2606 | C    | C2-N1-C1' | 6.79  | 126.27      | 118.80   |
| 51  | A2    | 1266 | G    | N7-C8-N9  | 6.79  | 116.49      | 113.10   |
| 51  | A2    | 4887 | C    | C6-N1-C2  | -6.79 | 117.59      | 120.30   |
| 51  | A2    | 1059 | C    | C6-N1-C2  | -6.78 | 117.59      | 120.30   |
| 52  | B1    | 1558 | C    | N1-C2-O2  | 6.77  | 122.96      | 118.90   |
| 51  | A2    | 219  | C    | N3-C2-O2  | -6.77 | 117.16      | 121.90   |
| 51  | A2    | 4886 | C    | C5-C6-N1  | 6.77  | 124.38      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 52  | B1    | 1520 | G    | N3-C4-N9   | 6.76  | 130.06      | 126.00   |
| 52  | B1    | 1032 | C    | C2-N1-C1'  | 6.76  | 126.23      | 118.80   |
| 52  | B1    | 1287 | A    | C2-N3-C4   | 6.75  | 113.98      | 110.60   |
| 52  | B1    | 814  | U    | N3-C2-O2   | -6.75 | 117.47      | 122.20   |
| 51  | A2    | 207  | C    | N3-C2-O2   | -6.75 | 117.18      | 121.90   |
| 51  | A2    | 649  | C    | N3-C2-O2   | -6.75 | 117.18      | 121.90   |
| 51  | A2    | 251  | G    | N3-C4-C5   | -6.74 | 125.23      | 128.60   |
| 51  | A2    | 1256 | G    | C4-N9-C1'  | 6.74  | 135.26      | 126.50   |
| 51  | A2    | 1989 | U    | C2-N1-C1'  | 6.74  | 125.78      | 117.70   |
| 16  | AK    | 78   | LEU  | CA-CB-CG   | 6.73  | 130.79      | 115.30   |
| 51  | A2    | 1746 | G    | N3-C4-C5   | -6.73 | 125.23      | 128.60   |
| 51  | A2    | 3890 | C    | N1-C2-O2   | 6.73  | 122.94      | 118.90   |
| 51  | A2    | 4464 | C    | N1-C2-O2   | 6.73  | 122.94      | 118.90   |
| 52  | B1    | 459  | C    | N1-C2-O2   | 6.73  | 122.94      | 118.90   |
| 51  | A2    | 1499 | G    | N3-C4-C5   | -6.72 | 125.24      | 128.60   |
| 51  | A2    | 216  | G    | N3-C2-N2   | -6.71 | 115.20      | 119.90   |
| 51  | A2    | 1576 | C    | C6-N1-C2   | -6.71 | 117.61      | 120.30   |
| 52  | B1    | 44   | U    | C2-N1-C1'  | 6.71  | 125.75      | 117.70   |
| 52  | B1    | 879  | C    | N3-C2-O2   | -6.70 | 117.21      | 121.90   |
| 51  | A2    | 4103 | C    | C6-N1-C2   | -6.69 | 117.62      | 120.30   |
| 51  | A2    | 1428 | U    | N1-C2-O2   | 6.69  | 127.48      | 122.80   |
| 83  | Bv    | 43   | C    | C5-C6-N1   | 6.69  | 124.34      | 121.00   |
| 51  | A2    | 4406 | C    | N1-C2-O2   | 6.69  | 122.91      | 118.90   |
| 52  | B1    | 879  | C    | C6-N1-C2   | -6.68 | 117.63      | 120.30   |
| 51  | A2    | 1564 | U    | N3-C2-O2   | -6.68 | 117.52      | 122.20   |
| 52  | B1    | 742  | U    | C5-C6-N1   | 6.68  | 126.04      | 122.70   |
| 83  | Bv    | 68   | C    | N1-C2-O2   | 6.68  | 122.91      | 118.90   |
| 51  | A2    | 2282 | C    | C6-N1-C2   | -6.68 | 117.63      | 120.30   |
| 51  | A2    | 6    | C    | C2-N1-C1'  | 6.67  | 126.14      | 118.80   |
| 52  | B1    | 1123 | C    | C6-N1-C2   | -6.67 | 117.63      | 120.30   |
| 51  | A2    | 2260 | U    | N3-C2-O2   | -6.67 | 117.53      | 122.20   |
| 52  | B1    | 67   | C    | N3-C2-O2   | -6.65 | 117.25      | 121.90   |
| 52  | B1    | 1156 | U    | N3-C2-O2   | -6.65 | 117.55      | 122.20   |
| 52  | B1    | 118  | C    | C6-N1-C1'  | -6.64 | 112.83      | 120.80   |
| 51  | A2    | 2840 | C    | N1-C2-O2   | 6.64  | 122.88      | 118.90   |
| 51  | A2    | 2727 | C    | N1-C2-O2   | 6.64  | 122.88      | 118.90   |
| 51  | A2    | 1638 | U    | N1-C2-O2   | 6.64  | 127.44      | 122.80   |
| 51  | A2    | 3882 | C    | C5-C6-N1   | 6.63  | 124.32      | 121.00   |
| 51  | A2    | 4088 | C    | N3-C2-O2   | -6.63 | 117.26      | 121.90   |
| 52  | B1    | 811  | A    | O4'-C1'-N9 | 6.63  | 113.51      | 108.20   |
| 51  | A2    | 2799 | C    | N3-C2-O2   | -6.62 | 117.27      | 121.90   |
| 8   | A4    | 14   | C    | N3-C2-O2   | -6.62 | 117.27      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 51  | A2    | 4886 | C    | C6-N1-C2  | -6.62 | 117.65      | 120.30   |
| 52  | B1    | 1117 | C    | C6-N1-C2  | -6.62 | 117.65      | 120.30   |
| 52  | B1    | 561  | A    | C4-N9-C1' | 6.61  | 138.21      | 126.30   |
| 51  | A2    | 4886 | C    | N3-C2-O2  | -6.61 | 117.28      | 121.90   |
| 52  | B1    | 1398 | G    | N3-C4-N9  | 6.60  | 129.96      | 126.00   |
| 51  | A2    | 4979 | C    | N1-C2-O2  | 6.60  | 122.86      | 118.90   |
| 51  | A2    | 2388 | U    | C6-N1-C1' | -6.59 | 111.97      | 121.20   |
| 51  | A2    | 907  | C    | N3-C2-O2  | -6.59 | 117.29      | 121.90   |
| 51  | A2    | 1746 | G    | C4-N9-C1' | 6.57  | 135.04      | 126.50   |
| 51  | A2    | 4406 | C    | N3-C2-O2  | -6.57 | 117.30      | 121.90   |
| 51  | A2    | 4729 | C    | N3-C2-O2  | -6.57 | 117.30      | 121.90   |
| 51  | A2    | 1193 | C    | N3-C2-O2  | -6.57 | 117.30      | 121.90   |
| 49  | At    | 106  | LEU  | CA-CB-CG  | 6.56  | 130.40      | 115.30   |
| 51  | A2    | 180  | C    | N3-C2-O2  | -6.56 | 117.31      | 121.90   |
| 51  | A2    | 4884 | C    | N3-C2-O2  | -6.56 | 117.31      | 121.90   |
| 52  | B1    | 496  | C    | N1-C2-O2  | 6.56  | 122.84      | 118.90   |
| 52  | B1    | 1591 | C    | N1-C2-O2  | 6.56  | 122.84      | 118.90   |
| 51  | A2    | 4489 | G    | N3-C4-C5  | -6.55 | 125.32      | 128.60   |
| 51  | A2    | 2400 | G    | C8-N9-C1' | -6.55 | 118.48      | 127.00   |
| 51  | A2    | 2751 | C    | C5-C6-N1  | 6.54  | 124.27      | 121.00   |
| 51  | A2    | 4519 | U    | N3-C2-O2  | -6.52 | 117.64      | 122.20   |
| 52  | B1    | 1557 | C    | N3-C2-O2  | -6.52 | 117.34      | 121.90   |
| 51  | A2    | 441  | C    | C5-C6-N1  | 6.51  | 124.26      | 121.00   |
| 51  | A2    | 1197 | C    | N1-C2-O2  | 6.51  | 122.81      | 118.90   |
| 51  | A2    | 119  | G    | C8-N9-C1' | -6.50 | 118.55      | 127.00   |
| 52  | B1    | 1156 | U    | N1-C2-O2  | 6.50  | 127.35      | 122.80   |
| 52  | B1    | 950  | C    | C6-N1-C2  | -6.49 | 117.70      | 120.30   |
| 52  | B1    | 918  | U    | N3-C2-O2  | -6.49 | 117.66      | 122.20   |
| 51  | A2    | 2260 | U    | N1-C2-O2  | 6.48  | 127.34      | 122.80   |
| 51  | A2    | 4007 | C    | C5-C6-N1  | 6.48  | 124.24      | 121.00   |
| 51  | A2    | 4979 | C    | N3-C2-O2  | -6.48 | 117.36      | 121.90   |
| 60  | BK    | 2    | LEU  | CA-CB-CG  | 6.47  | 130.19      | 115.30   |
| 51  | A2    | 4462 | U    | N3-C2-O2  | -6.47 | 117.67      | 122.20   |
| 51  | A2    | 2499 | C    | N3-C2-O2  | -6.47 | 117.37      | 121.90   |
| 51  | A2    | 4523 | C    | N1-C2-O2  | 6.47  | 122.78      | 118.90   |
| 51  | A2    | 1060 | C    | C6-N1-C2  | -6.46 | 117.71      | 120.30   |
| 51  | A2    | 2330 | C    | C6-N1-C2  | -6.46 | 117.72      | 120.30   |
| 51  | A2    | 1083 | U    | C2-N1-C1' | 6.46  | 125.45      | 117.70   |
| 51  | A2    | 4676 | C    | N3-C2-O2  | -6.46 | 117.38      | 121.90   |
| 51  | A2    | 1428 | U    | C2-N1-C1' | 6.45  | 125.44      | 117.70   |
| 51  | A2    | 901  | U    | P-O3'-C3' | 6.45  | 127.44      | 119.70   |
| 51  | A2    | 1789 | C    | C2-N1-C1' | 6.44  | 125.89      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 52  | B1    | 1254 | C    | O4'-C1'-N1 | 6.43  | 113.34      | 108.20   |
| 51  | A2    | 4834 | U    | C2-N3-C4   | 6.42  | 130.85      | 127.00   |
| 51  | A2    | 514  | C    | C6-N1-C2   | -6.42 | 117.73      | 120.30   |
| 51  | A2    | 5015 | C    | C2-N1-C1'  | 6.42  | 125.86      | 118.80   |
| 52  | B1    | 496  | C    | C2-N1-C1'  | 6.42  | 125.86      | 118.80   |
| 51  | A2    | 2646 | C    | N1-C2-O2   | 6.41  | 122.75      | 118.90   |
| 51  | A2    | 504  | U    | N1-C2-O2   | 6.41  | 127.29      | 122.80   |
| 51  | A2    | 668  | C    | C6-N1-C2   | -6.41 | 117.74      | 120.30   |
| 52  | B1    | 1288 | U    | C5-C6-N1   | 6.41  | 125.90      | 122.70   |
| 51  | A2    | 927  | C    | C6-N1-C2   | -6.40 | 117.74      | 120.30   |
| 52  | B1    | 1464 | C    | C6-N1-C1'  | -6.40 | 113.12      | 120.80   |
| 51  | A2    | 4409 | C    | C6-N1-C2   | -6.40 | 117.74      | 120.30   |
| 52  | B1    | 1286 | G    | N3-C4-C5   | -6.40 | 125.40      | 128.60   |
| 51  | A2    | 703  | C    | N3-C2-O2   | -6.39 | 117.42      | 121.90   |
| 52  | B1    | 833  | C    | C2-N1-C1'  | 6.38  | 125.82      | 118.80   |
| 52  | B1    | 67   | C    | C6-N1-C2   | -6.38 | 117.75      | 120.30   |
| 52  | B1    | 742  | U    | C2-N1-C1'  | 6.37  | 125.35      | 117.70   |
| 52  | B1    | 1237 | C    | N1-C2-O2   | 6.37  | 122.72      | 118.90   |
| 51  | A2    | 509  | C    | N1-C2-O2   | 6.37  | 122.72      | 118.90   |
| 52  | B1    | 620  | G    | N3-C4-N9   | 6.36  | 129.82      | 126.00   |
| 51  | A2    | 4834 | U    | C5-C6-N1   | 6.35  | 125.88      | 122.70   |
| 51  | A2    | 1350 | C    | N3-C2-O2   | -6.35 | 117.46      | 121.90   |
| 51  | A2    | 4151 | U    | C5-C6-N1   | 6.35  | 125.87      | 122.70   |
| 51  | A2    | 180  | C    | N3-C4-N4   | -6.35 | 113.56      | 118.00   |
| 52  | B1    | 797  | C    | P-O3'-C3'  | 6.35  | 127.32      | 119.70   |
| 52  | B1    | 325  | C    | N1-C2-O2   | 6.34  | 122.70      | 118.90   |
| 51  | A2    | 1947 | C    | C6-N1-C2   | -6.34 | 117.77      | 120.30   |
| 51  | A2    | 2686 | U    | N1-C2-O2   | 6.33  | 127.23      | 122.80   |
| 52  | B1    | 96   | C    | C6-N1-C1'  | -6.33 | 113.20      | 120.80   |
| 51  | A2    | 4676 | C    | N1-C2-O2   | 6.33  | 122.70      | 118.90   |
| 52  | B1    | 1120 | U    | N3-C2-O2   | -6.33 | 117.77      | 122.20   |
| 51  | A2    | 2879 | U    | N1-C2-O2   | 6.32  | 127.22      | 122.80   |
| 8   | A4    | 14   | C    | C6-N1-C2   | -6.31 | 117.78      | 120.30   |
| 52  | B1    | 89   | C    | N3-C2-O2   | -6.31 | 117.48      | 121.90   |
| 51  | A2    | 2840 | C    | C6-N1-C2   | -6.31 | 117.78      | 120.30   |
| 7   | A3    | 129  | C    | N3-C2-O2   | -6.30 | 117.49      | 121.90   |
| 51  | A2    | 1959 | C    | N3-C2-O2   | -6.30 | 117.49      | 121.90   |
| 52  | B1    | 89   | C    | C6-N1-C1'  | -6.30 | 113.24      | 120.80   |
| 51  | A2    | 727  | C    | N3-C2-O2   | -6.30 | 117.49      | 121.90   |
| 51  | A2    | 695  | C    | C6-N1-C2   | -6.29 | 117.78      | 120.30   |
| 51  | A2    | 119  | G    | N3-C4-C5   | -6.29 | 125.46      | 128.60   |
| 52  | B1    | 918  | U    | C2-N1-C1'  | 6.29  | 125.25      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 52  | B1    | 1261 | C    | N3-C2-O2   | -6.28 | 117.50      | 121.90   |
| 51  | A2    | 1653 | U    | N1-C2-O2   | 6.28  | 127.20      | 122.80   |
| 52  | B1    | 632  | C    | C2-N1-C1'  | 6.28  | 125.71      | 118.80   |
| 51  | A2    | 4255 | U    | N3-C2-O2   | -6.27 | 117.81      | 122.20   |
| 51  | A2    | 918  | C    | N3-C2-O2   | -6.27 | 117.51      | 121.90   |
| 52  | B1    | 173  | A    | N9-C1'-C2' | -6.27 | 105.10      | 112.00   |
| 52  | B1    | 797  | C    | OP2-P-O3'  | 6.27  | 118.99      | 105.20   |
| 51  | A2    | 163  | C    | C2-N1-C1'  | 6.26  | 125.69      | 118.80   |
| 51  | A2    | 493  | G    | C8-N9-C1'  | -6.26 | 118.86      | 127.00   |
| 52  | B1    | 1267 | C    | C2-N1-C1'  | 6.26  | 125.68      | 118.80   |
| 52  | B1    | 1117 | C    | N1-C2-O2   | 6.25  | 122.65      | 118.90   |
| 51  | A2    | 1930 | U    | C2-N1-C1'  | 6.25  | 125.20      | 117.70   |
| 52  | B1    | 1398 | G    | C6-C5-N7   | -6.25 | 126.65      | 130.40   |
| 51  | A2    | 3880 | C    | N3-C2-O2   | -6.25 | 117.52      | 121.90   |
| 52  | B1    | 96   | C    | C6-N1-C2   | -6.24 | 117.80      | 120.30   |
| 51  | A2    | 3853 | C    | C2-N1-C1'  | 6.23  | 125.65      | 118.80   |
| 7   | A3    | 99   | U    | C2-N1-C1'  | 6.23  | 125.17      | 117.70   |
| 51  | A2    | 3880 | C    | C6-N1-C2   | -6.23 | 117.81      | 120.30   |
| 51  | A2    | 4881 | C    | C6-N1-C2   | -6.23 | 117.81      | 120.30   |
| 52  | B1    | 570  | C    | N1-C2-O2   | 6.22  | 122.63      | 118.90   |
| 51  | A2    | 4462 | U    | C2-N1-C1'  | 6.22  | 125.16      | 117.70   |
| 7   | A3    | 126  | C    | C6-N1-C1'  | -6.21 | 113.35      | 120.80   |
| 51  | A2    | 4088 | C    | C6-N1-C2   | -6.21 | 117.82      | 120.30   |
| 52  | B1    | 1586 | U    | N3-C2-O2   | -6.20 | 117.86      | 122.20   |
| 51  | A2    | 2727 | C    | N3-C2-O2   | -6.20 | 117.56      | 121.90   |
| 52  | B1    | 1237 | C    | C6-N1-C2   | -6.20 | 117.82      | 120.30   |
| 52  | B1    | 570  | C    | N3-C2-O2   | -6.19 | 117.56      | 121.90   |
| 51  | A2    | 911  | C    | N3-C2-O2   | -6.19 | 117.57      | 121.90   |
| 51  | A2    | 4011 | C    | N3-C2-O2   | -6.19 | 117.57      | 121.90   |
| 52  | B1    | 1472 | C    | C2-N1-C1'  | 6.18  | 125.60      | 118.80   |
| 52  | B1    | 578  | C    | N1-C2-O2   | 6.18  | 122.61      | 118.90   |
| 51  | A2    | 493  | G    | N3-C4-N9   | 6.18  | 129.71      | 126.00   |
| 51  | A2    | 2344 | C    | C6-N1-C2   | -6.18 | 117.83      | 120.30   |
| 51  | A2    | 2389 | C    | C6-N1-C2   | -6.18 | 117.83      | 120.30   |
| 52  | B1    | 804  | U    | N1-C2-O2   | 6.18  | 127.12      | 122.80   |
| 51  | A2    | 251  | G    | N3-C4-N9   | 6.17  | 129.70      | 126.00   |
| 84  | Bx    | 46   | U    | N3-C2-O2   | -6.17 | 117.88      | 122.20   |
| 51  | A2    | 1576 | C    | C6-N1-C1'  | -6.17 | 113.40      | 120.80   |
| 7   | A3    | 126  | C    | C6-N1-C2   | -6.17 | 117.83      | 120.30   |
| 51  | A2    | 504  | U    | C2-N1-C1'  | 6.16  | 125.10      | 117.70   |
| 51  | A2    | 958  | U    | N1-C2-O2   | 6.16  | 127.11      | 122.80   |
| 51  | A2    | 1874 | C    | N1-C2-O2   | 6.16  | 122.60      | 118.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 51  | A2    | 1176 | C    | N1-C2-O2   | 6.16  | 122.60      | 118.90   |
| 51  | A2    | 4042 | C    | C2-N1-C1'  | 6.16  | 125.58      | 118.80   |
| 51  | A2    | 2822 | U    | N3-C2-O2   | -6.16 | 117.89      | 122.20   |
| 52  | B1    | 210  | U    | C2-N1-C1'  | 6.16  | 125.09      | 117.70   |
| 51  | A2    | 77   | U    | N1-C2-O2   | 6.15  | 127.10      | 122.80   |
| 52  | B1    | 4    | C    | C2-N1-C1'  | 6.15  | 125.56      | 118.80   |
| 52  | B1    | 1714 | U    | C2-N1-C1'  | 6.14  | 125.07      | 117.70   |
| 51  | A2    | 2800 | U    | N1-C2-O2   | 6.14  | 127.10      | 122.80   |
| 51  | A2    | 2835 | C    | N1-C2-O2   | 6.13  | 122.58      | 118.90   |
| 52  | B1    | 742  | U    | C6-N1-C2   | -6.13 | 117.32      | 121.00   |
| 52  | B1    | 1286 | G    | C8-N9-C1'  | -6.13 | 119.03      | 127.00   |
| 51  | A2    | 4946 | U    | P-O3'-C3'  | 6.13  | 127.05      | 119.70   |
| 52  | B1    | 1520 | G    | C8-N9-C1'  | -6.12 | 119.05      | 127.00   |
| 51  | A2    | 4880 | C    | N1-C2-O2   | 6.11  | 122.57      | 118.90   |
| 51  | A2    | 4042 | C    | C6-N1-C2   | -6.11 | 117.86      | 120.30   |
| 51  | A2    | 3572 | C    | C2-N1-C1'  | 6.10  | 125.51      | 118.80   |
| 51  | A2    | 1702 | C    | N1-C2-O2   | 6.10  | 122.56      | 118.90   |
| 51  | A2    | 645  | C    | C5-C6-N1   | 6.10  | 124.05      | 121.00   |
| 51  | A2    | 4276 | C    | C2-N1-C1'  | 6.09  | 125.50      | 118.80   |
| 52  | B1    | 1117 | C    | O4'-C1'-N1 | 6.09  | 113.07      | 108.20   |
| 51  | A2    | 4707 | G    | N7-C8-N9   | 6.09  | 116.15      | 113.10   |
| 51  | A2    | 671  | C    | N3-C2-O2   | -6.09 | 117.64      | 121.90   |
| 51  | A2    | 4676 | C    | C6-N1-C2   | -6.09 | 117.86      | 120.30   |
| 52  | B1    | 1554 | C    | C6-N1-C2   | -6.09 | 117.86      | 120.30   |
| 51  | A2    | 4169 | C    | C6-N1-C2   | -6.09 | 117.86      | 120.30   |
| 52  | B1    | 67   | C    | C5-C6-N1   | 6.08  | 124.04      | 121.00   |
| 52  | B1    | 568  | C    | C2-N1-C1'  | 6.08  | 125.49      | 118.80   |
| 51  | A2    | 905  | G    | N3-C2-N2   | -6.08 | 115.64      | 119.90   |
| 51  | A2    | 1193 | C    | C6-N1-C2   | -6.08 | 117.87      | 120.30   |
| 52  | B1    | 106  | C    | C2-N1-C1'  | 6.08  | 125.49      | 118.80   |
| 52  | B1    | 210  | U    | C5-C6-N1   | 6.08  | 125.74      | 122.70   |
| 51  | A2    | 219  | C    | O4'-C1'-N1 | 6.08  | 113.06      | 108.20   |
| 51  | A2    | 3890 | C    | N3-C2-O2   | -6.07 | 117.65      | 121.90   |
| 52  | B1    | 1019 | C    | C6-N1-C2   | -6.07 | 117.87      | 120.30   |
| 51  | A2    | 645  | C    | N1-C2-O2   | 6.07  | 122.54      | 118.90   |
| 52  | B1    | 490  | C    | C6-N1-C2   | -6.07 | 117.87      | 120.30   |
| 8   | A4    | 19   | C    | N1-C2-O2   | 6.06  | 122.54      | 118.90   |
| 84  | Bx    | 46   | U    | N1-C2-O2   | 6.06  | 127.04      | 122.80   |
| 51  | A2    | 1499 | G    | N3-C4-N9   | 6.05  | 129.63      | 126.00   |
| 51  | A2    | 4464 | C    | N3-C2-O2   | -6.05 | 117.67      | 121.90   |
| 51  | A2    | 149  | U    | O4'-C1'-N1 | 6.05  | 113.04      | 108.20   |
| 51  | A2    | 4489 | G    | C8-N9-C1'  | -6.05 | 119.14      | 127.00   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 52  | B1    | 621  | C    | C6-N1-C2  | -6.05 | 117.88      | 120.30   |
| 52  | B1    | 1811 | C    | C6-N1-C1' | -6.04 | 113.55      | 120.80   |
| 52  | B1    | 1425 | G    | N3-C4-N9  | 6.04  | 129.62      | 126.00   |
| 51  | A2    | 1607 | G    | C4-N9-C1' | 6.04  | 134.35      | 126.50   |
| 52  | B1    | 1520 | G    | C8-N9-C4  | -6.04 | 103.99      | 106.40   |
| 51  | A2    | 1713 | C    | C2-N1-C1' | 6.03  | 125.44      | 118.80   |
| 51  | A2    | 698  | C    | C2-N1-C1' | 6.03  | 125.44      | 118.80   |
| 51  | A2    | 2879 | U    | N3-C2-O2  | -6.03 | 117.98      | 122.20   |
| 51  | A2    | 703  | C    | C2-N1-C1' | 6.02  | 125.43      | 118.80   |
| 51  | A2    | 2064 | C    | C6-N1-C2  | -6.02 | 117.89      | 120.30   |
| 51  | A2    | 1500 | A    | P-O3'-C3' | 6.02  | 126.92      | 119.70   |
| 51  | A2    | 2800 | U    | N3-C2-O2  | -6.01 | 117.99      | 122.20   |
| 52  | B1    | 1425 | G    | C4-N9-C1' | 6.01  | 134.31      | 126.50   |
| 51  | A2    | 2325 | C    | C6-N1-C1' | -6.00 | 113.59      | 120.80   |
| 52  | B1    | 1032 | C    | C6-N1-C2  | -6.00 | 117.90      | 120.30   |
| 51  | A2    | 4406 | C    | C6-N1-C2  | -5.99 | 117.90      | 120.30   |
| 51  | A2    | 471  | C    | C6-N1-C2  | -5.99 | 117.91      | 120.30   |
| 51  | A2    | 927  | C    | N1-C2-O2  | 5.99  | 122.49      | 118.90   |
| 52  | B1    | 621  | C    | C6-N1-C1' | -5.98 | 113.62      | 120.80   |
| 83  | Bv    | 73   | A    | P-O3'-C3' | 5.98  | 126.88      | 119.70   |
| 51  | A2    | 2686 | U    | N3-C2-O2  | -5.98 | 118.01      | 122.20   |
| 52  | B1    | 1590 | C    | C6-N1-C2  | -5.98 | 117.91      | 120.30   |
| 51  | A2    | 4523 | C    | N3-C2-O2  | -5.97 | 117.72      | 121.90   |
| 51  | A2    | 1193 | C    | C2-N1-C1' | 5.97  | 125.37      | 118.80   |
| 83  | Bv    | 62   | C    | N1-C2-O2  | 5.97  | 122.48      | 118.90   |
| 51  | A2    | 50   | C    | N1-C2-O2  | 5.97  | 122.48      | 118.90   |
| 51  | A2    | 2398 | C    | C6-N1-C1' | -5.97 | 113.64      | 120.80   |
| 52  | B1    | 526  | A    | C8-N9-C4  | -5.97 | 103.41      | 105.80   |
| 51  | A2    | 1466 | G    | C8-N9-C1' | -5.96 | 119.25      | 127.00   |
| 51  | A2    | 4946 | U    | OP1-P-O3' | 5.96  | 118.31      | 105.20   |
| 51  | A2    | 2751 | C    | C2-N1-C1' | 5.96  | 125.36      | 118.80   |
| 51  | A2    | 3664 | U    | C2-N1-C1' | 5.96  | 124.85      | 117.70   |
| 52  | B1    | 67   | C    | C2-N3-C4  | 5.95  | 122.87      | 119.90   |
| 51  | A2    | 509  | C    | C2-N1-C1' | 5.94  | 125.33      | 118.80   |
| 52  | B1    | 1517 | G    | N3-C4-N9  | -5.94 | 122.44      | 126.00   |
| 52  | B1    | 1750 | C    | C2-N1-C1' | 5.94  | 125.33      | 118.80   |
| 52  | B1    | 67   | C    | C6-N1-C1' | -5.93 | 113.68      | 120.80   |
| 51  | A2    | 1959 | C    | C6-N1-C2  | -5.93 | 117.93      | 120.30   |
| 51  | A2    | 898  | U    | N1-C2-O2  | 5.93  | 126.95      | 122.80   |
| 51  | A2    | 71   | C    | P-O3'-C3' | 5.92  | 126.81      | 119.70   |
| 52  | B1    | 804  | U    | C2-N1-C1' | 5.92  | 124.80      | 117.70   |
| 51  | A2    | 219  | C    | C6-N1-C1' | -5.92 | 113.70      | 120.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 51  | A2    | 4276 | C    | C6-N1-C2   | -5.91 | 117.94      | 120.30   |
| 51  | A2    | 695  | C    | N1-C2-O2   | 5.91  | 122.45      | 118.90   |
| 51  | A2    | 727  | C    | N1-C2-O2   | 5.90  | 122.44      | 118.90   |
| 8   | A4    | 78   | C    | C2-N1-C1'  | 5.90  | 125.29      | 118.80   |
| 51  | A2    | 252  | C    | N1-C2-O2   | 5.89  | 122.44      | 118.90   |
| 52  | B1    | 1117 | C    | C2-N1-C1'  | 5.89  | 125.28      | 118.80   |
| 52  | B1    | 100  | U    | N1-C2-O2   | 5.89  | 126.92      | 122.80   |
| 52  | B1    | 1271 | C    | C6-N1-C2   | -5.89 | 117.94      | 120.30   |
| 51  | A2    | 4633 | C    | N1-C2-O2   | 5.89  | 122.43      | 118.90   |
| 52  | B1    | 186  | C    | C6-N1-C2   | -5.88 | 117.95      | 120.30   |
| 51  | A2    | 4443 | U    | C2-N1-C1'  | 5.88  | 124.76      | 117.70   |
| 51  | A2    | 214  | C    | N1-C2-O2   | 5.88  | 122.43      | 118.90   |
| 51  | A2    | 4545 | C    | N3-C2-O2   | -5.88 | 117.78      | 121.90   |
| 51  | A2    | 4824 | C    | N1-C2-O2   | 5.88  | 122.43      | 118.90   |
| 52  | B1    | 1554 | C    | P-O3'-C3'  | 5.87  | 126.75      | 119.70   |
| 51  | A2    | 891  | C    | C5-C6-N1   | 5.87  | 123.94      | 121.00   |
| 8   | A4    | 29   | C    | C6-N1-C2   | -5.87 | 117.95      | 120.30   |
| 51  | A2    | 2398 | C    | C5-C6-N1   | 5.87  | 123.93      | 121.00   |
| 51  | A2    | 2256 | C    | C2-N1-C1'  | 5.87  | 125.25      | 118.80   |
| 51  | A2    | 2840 | C    | C2-N1-C1'  | 5.87  | 125.25      | 118.80   |
| 52  | B1    | 1156 | U    | C2-N1-C1'  | 5.87  | 124.74      | 117.70   |
| 83  | Bv    | 68   | C    | N3-C2-O2   | -5.84 | 117.81      | 121.90   |
| 51  | A2    | 1966 | G    | N3-C4-C5   | -5.84 | 125.68      | 128.60   |
| 52  | B1    | 15   | U    | C5-C6-N1   | 5.84  | 125.62      | 122.70   |
| 52  | B1    | 89   | C    | C6-N1-C2   | -5.84 | 117.97      | 120.30   |
| 52  | B1    | 1557 | C    | C6-N1-C2   | -5.83 | 117.97      | 120.30   |
| 51  | A2    | 4519 | U    | N1-C2-O2   | 5.82  | 126.88      | 122.80   |
| 52  | B1    | 1472 | C    | N3-C2-O2   | -5.82 | 117.83      | 121.90   |
| 51  | A2    | 2000 | C    | N3-C2-O2   | -5.82 | 117.83      | 121.90   |
| 51  | A2    | 4327 | C    | C2-N1-C1'  | 5.82  | 125.20      | 118.80   |
| 51  | A2    | 251  | G    | C8-N9-C1'  | -5.81 | 119.44      | 127.00   |
| 51  | A2    | 2473 | U    | N3-C2-O2   | -5.81 | 118.13      | 122.20   |
| 52  | B1    | 632  | C    | C6-N1-C2   | -5.80 | 117.98      | 120.30   |
| 51  | A2    | 907  | C    | N1-C2-O2   | 5.80  | 122.38      | 118.90   |
| 52  | B1    | 44   | U    | N1-C2-O2   | 5.80  | 126.86      | 122.80   |
| 51  | A2    | 504  | U    | C5-C6-N1   | 5.80  | 125.60      | 122.70   |
| 52  | B1    | 1163 | C    | N1-C2-O2   | 5.80  | 122.38      | 118.90   |
| 52  | B1    | 915  | G    | O4'-C1'-N9 | 5.80  | 112.84      | 108.20   |
| 52  | B1    | 950  | C    | N1-C2-O2   | 5.79  | 122.38      | 118.90   |
| 84  | Bx    | 46   | U    | C2-N1-C1'  | 5.79  | 124.65      | 117.70   |
| 52  | B1    | 325  | C    | C2-N1-C1'  | 5.79  | 125.17      | 118.80   |
| 51  | A2    | 2646 | C    | N3-C2-O2   | -5.79 | 117.85      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 51  | A2    | 5015 | C    | C6-N1-C2  | -5.79 | 117.99      | 120.30   |
| 83  | Bv    | 43   | C    | C2-N3-C4  | 5.79  | 122.79      | 119.90   |
| 79  | Bd    | 30   | LEU  | CA-CB-CG  | 5.78  | 128.60      | 115.30   |
| 52  | B1    | 1364 | U    | N1-C2-O2  | 5.78  | 126.85      | 122.80   |
| 7   | A3    | 96   | C    | N3-C2-O2  | -5.78 | 117.85      | 121.90   |
| 52  | B1    | 1053 | C    | C6-N1-C2  | -5.78 | 117.99      | 120.30   |
| 51  | A2    | 3725 | G    | N9-C4-C5  | 5.78  | 107.71      | 105.40   |
| 7   | A3    | 99   | U    | N3-C2-O2  | -5.77 | 118.16      | 122.20   |
| 51  | A2    | 3903 | U    | N3-C2-O2  | -5.77 | 118.16      | 122.20   |
| 52  | B1    | 1121 | G    | C4-N9-C1' | 5.76  | 133.99      | 126.50   |
| 51  | A2    | 4834 | U    | N1-C2-O2  | 5.76  | 126.83      | 122.80   |
| 51  | A2    | 509  | C    | C6-N1-C2  | -5.76 | 118.00      | 120.30   |
| 51  | A2    | 4824 | C    | N3-C2-O2  | -5.76 | 117.87      | 121.90   |
| 52  | B1    | 1102 | G    | N3-C2-N2  | -5.75 | 115.87      | 119.90   |
| 51  | A2    | 2499 | C    | C6-N1-C2  | -5.75 | 118.00      | 120.30   |
| 51  | A2    | 2664 | C    | C6-N1-C2  | -5.75 | 118.00      | 120.30   |
| 51  | A2    | 4107 | C    | P-O3'-C3' | 5.75  | 126.60      | 119.70   |
| 51  | A2    | 4602 | C    | N3-C2-O2  | -5.75 | 117.88      | 121.90   |
| 51  | A2    | 3759 | C    | C2-N1-C1' | 5.75  | 125.12      | 118.80   |
| 52  | B1    | 298  | G    | N3-C4-N9  | 5.75  | 129.45      | 126.00   |
| 51  | A2    | 1284 | C    | C5-C6-N1  | 5.75  | 123.87      | 121.00   |
| 52  | B1    | 178  | C    | N1-C2-O2  | 5.74  | 122.35      | 118.90   |
| 51  | A2    | 276  | C    | N1-C2-O2  | 5.74  | 122.34      | 118.90   |
| 51  | A2    | 3881 | C    | C6-N1-C2  | -5.74 | 118.00      | 120.30   |
| 52  | B1    | 738  | C    | N1-C2-O2  | 5.74  | 122.34      | 118.90   |
| 52  | B1    | 119  | U    | C2-N1-C1' | 5.74  | 124.58      | 117.70   |
| 51  | A2    | 4011 | C    | C2-N1-C1' | 5.73  | 125.11      | 118.80   |
| 7   | A3    | 57   | C    | N3-C2-O2  | -5.73 | 117.89      | 121.90   |
| 51  | A2    | 647  | U    | C2-N1-C1' | 5.73  | 124.58      | 117.70   |
| 52  | B1    | 1690 | U    | C2-N1-C1' | 5.73  | 124.58      | 117.70   |
| 52  | B1    | 1811 | C    | N1-C2-O2  | 5.73  | 122.34      | 118.90   |
| 52  | B1    | 592  | C    | N1-C2-O2  | 5.72  | 122.33      | 118.90   |
| 51  | A2    | 1930 | U    | N3-C2-O2  | -5.72 | 118.19      | 122.20   |
| 51  | A2    | 1059 | C    | C2-N1-C1' | 5.72  | 125.09      | 118.80   |
| 51  | A2    | 3864 | C    | C6-N1-C2  | -5.71 | 118.01      | 120.30   |
| 51  | A2    | 1255 | C    | C6-N1-C2  | -5.71 | 118.02      | 120.30   |
| 51  | A2    | 2389 | C    | N1-C2-O2  | 5.71  | 122.33      | 118.90   |
| 52  | B1    | 1364 | U    | N3-C2-O2  | -5.71 | 118.20      | 122.20   |
| 51  | A2    | 695  | C    | C2-N1-C1' | 5.71  | 125.08      | 118.80   |
| 51  | A2    | 2473 | U    | N1-C2-O2  | 5.70  | 126.79      | 122.80   |
| 52  | B1    | 638  | C    | C2-N1-C1' | 5.69  | 125.06      | 118.80   |
| 52  | B1    | 179  | C    | N3-C2-O2  | -5.69 | 117.92      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 51  | A2    | 1576 | C    | O4'-C1'-N1 | 5.69  | 112.75      | 108.20   |
| 51  | A2    | 2742 | U    | O4'-C1'-N1 | 5.69  | 112.75      | 108.20   |
| 51  | A2    | 1874 | C    | N3-C2-O2   | -5.68 | 117.92      | 121.90   |
| 51  | A2    | 1737 | C    | N1-C2-O2   | 5.68  | 122.31      | 118.90   |
| 51  | A2    | 4909 | G    | C8-N9-C1'  | -5.68 | 119.62      | 127.00   |
| 52  | B1    | 174  | C    | C5-C6-N1   | 5.68  | 123.84      | 121.00   |
| 51  | A2    | 242  | C    | C6-N1-C2   | -5.67 | 118.03      | 120.30   |
| 52  | B1    | 561  | A    | C8-N9-C1'  | -5.67 | 117.49      | 127.70   |
| 52  | B1    | 526  | A    | N7-C8-N9   | 5.67  | 116.64      | 113.80   |
| 51  | A2    | 703  | C    | C6-N1-C2   | -5.67 | 118.03      | 120.30   |
| 8   | A4    | 92   | C    | C6-N1-C2   | -5.67 | 118.03      | 120.30   |
| 51  | A2    | 4010 | C    | C6-N1-C2   | -5.67 | 118.03      | 120.30   |
| 51  | A2    | 2308 | U    | N3-C2-O2   | -5.66 | 118.24      | 122.20   |
| 52  | B1    | 106  | C    | N1-C2-O2   | 5.66  | 122.30      | 118.90   |
| 52  | B1    | 487  | U    | N3-C2-O2   | -5.66 | 118.24      | 122.20   |
| 52  | B1    | 1472 | C    | N1-C2-O2   | 5.66  | 122.30      | 118.90   |
| 52  | B1    | 324  | C    | C6-N1-C2   | -5.65 | 118.04      | 120.30   |
| 83  | Bv    | 20   | U    | C6-N1-C1'  | -5.65 | 113.29      | 121.20   |
| 51  | A2    | 3863 | U    | N1-C2-O2   | 5.65  | 126.75      | 122.80   |
| 52  | B1    | 1523 | C    | N1-C2-O2   | 5.65  | 122.29      | 118.90   |
| 51  | A2    | 516  | C    | C5-C6-N1   | 5.65  | 123.82      | 121.00   |
| 51  | A2    | 4728 | C    | C6-N1-C2   | -5.65 | 118.04      | 120.30   |
| 51  | A2    | 1966 | G    | C8-N9-C1'  | -5.64 | 119.66      | 127.00   |
| 51  | A2    | 2418 | G    | C4-N9-C1'  | 5.64  | 133.84      | 126.50   |
| 8   | A4    | 78   | C    | C6-N1-C2   | -5.64 | 118.05      | 120.30   |
| 51  | A2    | 2389 | C    | C6-N1-C1'  | -5.64 | 114.03      | 120.80   |
| 52  | B1    | 1852 | C    | C2-N1-C1'  | 5.64  | 125.00      | 118.80   |
| 51  | A2    | 2840 | C    | N3-C2-O2   | -5.63 | 117.96      | 121.90   |
| 52  | B1    | 1261 | C    | N1-C2-O2   | 5.63  | 122.28      | 118.90   |
| 51  | A2    | 4880 | C    | N3-C2-O2   | -5.62 | 117.97      | 121.90   |
| 52  | B1    | 814  | U    | N1-C2-O2   | 5.62  | 126.73      | 122.80   |
| 52  | B1    | 1398 | G    | N3-C4-C5   | -5.62 | 125.79      | 128.60   |
| 51  | A2    | 4909 | G    | C4-N9-C1'  | 5.62  | 133.80      | 126.50   |
| 51  | A2    | 2727 | C    | C6-N1-C1'  | -5.61 | 114.06      | 120.80   |
| 51  | A2    | 276  | C    | N3-C2-O2   | -5.60 | 117.98      | 121.90   |
| 52  | B1    | 295  | C    | C5-C6-N1   | 5.60  | 123.80      | 121.00   |
| 52  | B1    | 1064 | C    | C6-N1-C2   | -5.59 | 118.06      | 120.30   |
| 51  | A2    | 219  | C    | C5-C6-N1   | 5.59  | 123.80      | 121.00   |
| 51  | A2    | 4270 | C    | N1-C2-O2   | 5.59  | 122.25      | 118.90   |
| 51  | A2    | 2871 | C    | C2-N1-C1'  | 5.59  | 124.95      | 118.80   |
| 51  | A2    | 1746 | G    | C8-N9-C1'  | -5.59 | 119.74      | 127.00   |
| 51  | A2    | 4878 | C    | N1-C2-O2   | 5.59  | 122.25      | 118.90   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 52  | B1    | 402  | C    | N3-C2-O2  | -5.58 | 117.99      | 121.90   |
| 51  | A2    | 2363 | U    | C2-N1-C1' | 5.58  | 124.40      | 117.70   |
| 52  | B1    | 1425 | G    | C8-N9-C1' | -5.58 | 119.75      | 127.00   |
| 51  | A2    | 695  | C    | N3-C2-O2  | -5.58 | 118.00      | 121.90   |
| 51  | A2    | 1259 | C    | C5-C6-N1  | 5.58  | 123.79      | 121.00   |
| 83  | Bv    | 2    | C    | C2-N1-C1' | 5.58  | 124.93      | 118.80   |
| 8   | A4    | 19   | C    | C2-N1-C1' | 5.57  | 124.93      | 118.80   |
| 51  | A2    | 242  | C    | N1-C2-O2  | 5.57  | 122.24      | 118.90   |
| 52  | B1    | 620  | G    | C4-N9-C1' | 5.57  | 133.74      | 126.50   |
| 51  | A2    | 637  | C    | N1-C2-O2  | 5.57  | 122.24      | 118.90   |
| 51  | A2    | 4856 | G    | N3-C4-N9  | 5.57  | 129.34      | 126.00   |
| 51  | A2    | 4881 | C    | C2-N1-C1' | 5.57  | 124.92      | 118.80   |
| 7   | A3    | 126  | C    | C5-C6-N1  | 5.57  | 123.78      | 121.00   |
| 51  | A2    | 2511 | C    | C2-N1-C1' | 5.57  | 124.92      | 118.80   |
| 52  | B1    | 1558 | C    | N3-C2-O2  | -5.56 | 118.00      | 121.90   |
| 52  | B1    | 1714 | U    | C5-C6-N1  | 5.56  | 125.48      | 122.70   |
| 51  | A2    | 242  | C    | N3-C2-O2  | -5.55 | 118.01      | 121.90   |
| 51  | A2    | 1564 | U    | C6-N1-C1' | -5.55 | 113.42      | 121.20   |
| 51  | A2    | 1259 | C    | N3-C2-O2  | -5.55 | 118.01      | 121.90   |
| 51  | A2    | 2029 | U    | N3-C2-O2  | -5.55 | 118.31      | 122.20   |
| 51  | A2    | 4250 | C    | N3-C2-O2  | -5.55 | 118.01      | 121.90   |
| 51  | A2    | 4327 | C    | C6-N1-C2  | -5.55 | 118.08      | 120.30   |
| 52  | B1    | 1237 | C    | N3-C2-O2  | -5.55 | 118.01      | 121.90   |
| 52  | B1    | 298  | G    | C4-N9-C1' | 5.55  | 133.72      | 126.50   |
| 51  | A2    | 4880 | C    | C6-N1-C2  | -5.55 | 118.08      | 120.30   |
| 52  | B1    | 797  | C    | C5-C6-N1  | 5.55  | 123.77      | 121.00   |
| 52  | B1    | 1811 | C    | C5-C6-N1  | 5.55  | 123.77      | 121.00   |
| 52  | B1    | 496  | C    | N3-C2-O2  | -5.54 | 118.02      | 121.90   |
| 51  | A2    | 4191 | U    | N3-C2-O2  | -5.54 | 118.32      | 122.20   |
| 52  | B1    | 314  | U    | N3-C2-O2  | -5.54 | 118.32      | 122.20   |
| 16  | AK    | 54   | LEU  | CA-CB-CG  | 5.54  | 128.03      | 115.30   |
| 52  | B1    | 386  | C    | N1-C2-O2  | 5.54  | 122.22      | 118.90   |
| 51  | A2    | 1773 | U    | N3-C2-O2  | -5.53 | 118.33      | 122.20   |
| 52  | B1    | 797  | C    | N1-C2-O2  | 5.53  | 122.22      | 118.90   |
| 51  | A2    | 1561 | C    | C6-N1-C2  | -5.53 | 118.09      | 120.30   |
| 51  | A2    | 276  | C    | C6-N1-C2  | -5.52 | 118.09      | 120.30   |
| 52  | B1    | 1600 | G    | C4-N9-C1' | 5.52  | 133.68      | 126.50   |
| 51  | A2    | 1756 | C    | N1-C2-O2  | 5.52  | 122.21      | 118.90   |
| 51  | A2    | 4011 | C    | C6-N1-C2  | -5.52 | 118.09      | 120.30   |
| 52  | B1    | 1600 | G    | N3-C4-C5  | -5.52 | 125.84      | 128.60   |
| 51  | A2    | 4884 | C    | C5-C6-N1  | 5.52  | 123.76      | 121.00   |
| 52  | B1    | 741  | C    | N1-C2-O2  | 5.52  | 122.21      | 118.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 51  | A2    | 2373 | G    | C8-N9-C1'  | -5.51 | 119.84      | 127.00   |
| 51  | A2    | 3903 | U    | N1-C2-O2   | 5.51  | 126.66      | 122.80   |
| 52  | B1    | 739  | C    | N1-C2-O2   | 5.51  | 122.21      | 118.90   |
| 83  | Bv    | 73   | A    | O3'-P-O5'  | 5.51  | 114.47      | 104.00   |
| 52  | B1    | 89   | C    | O4'-C1'-N1 | 5.51  | 112.61      | 108.20   |
| 51  | A2    | 962  | C    | N1-C2-O2   | 5.50  | 122.20      | 118.90   |
| 51  | A2    | 4881 | C    | N1-C2-O2   | 5.50  | 122.20      | 118.90   |
| 52  | B1    | 804  | U    | N3-C2-O2   | -5.50 | 118.35      | 122.20   |
| 51  | A2    | 4881 | C    | C5-C6-N1   | 5.50  | 123.75      | 121.00   |
| 52  | B1    | 839  | C    | C6-N1-C2   | -5.50 | 118.10      | 120.30   |
| 51  | A2    | 2829 | A    | C8-N9-C4   | -5.49 | 103.60      | 105.80   |
| 51  | A2    | 3824 | U    | N3-C2-O2   | -5.49 | 118.36      | 122.20   |
| 51  | A2    | 2373 | G    | N7-C8-N9   | 5.49  | 115.84      | 113.10   |
| 51  | A2    | 2389 | C    | C5-C6-N1   | 5.49  | 123.75      | 121.00   |
| 51  | A2    | 3759 | C    | N3-C2-O2   | -5.49 | 118.06      | 121.90   |
| 51  | A2    | 4826 | G    | N3-C2-N2   | -5.49 | 116.06      | 119.90   |
| 52  | B1    | 459  | C    | N3-C2-O2   | -5.49 | 118.06      | 121.90   |
| 51  | A2    | 40   | G    | N7-C8-N9   | 5.49  | 115.84      | 113.10   |
| 52  | B1    | 189  | U    | N1-C2-O2   | 5.49  | 126.64      | 122.80   |
| 51  | A2    | 4007 | C    | C6-N1-C2   | -5.48 | 118.11      | 120.30   |
| 51  | A2    | 2800 | U    | C2-N1-C1'  | 5.48  | 124.28      | 117.70   |
| 83  | Bv    | 25   | C    | C6-N1-C2   | -5.48 | 118.11      | 120.30   |
| 51  | A2    | 4545 | C    | N1-C2-O2   | 5.48  | 122.19      | 118.90   |
| 51  | A2    | 2365 | U    | C5-C6-N1   | 5.48  | 125.44      | 122.70   |
| 52  | B1    | 1120 | U    | N1-C2-O2   | 5.48  | 126.63      | 122.80   |
| 51  | A2    | 450  | C    | C6-N1-C2   | -5.47 | 118.11      | 120.30   |
| 51  | A2    | 463  | C    | C6-N1-C2   | -5.47 | 118.11      | 120.30   |
| 51  | A2    | 941  | C    | C6-N1-C2   | -5.47 | 118.11      | 120.30   |
| 51  | A2    | 1083 | U    | N3-C2-O2   | -5.47 | 118.37      | 122.20   |
| 52  | B1    | 1551 | U    | C6-N1-C1'  | -5.47 | 113.53      | 121.20   |
| 51  | A2    | 927  | C    | C5-C6-N1   | 5.47  | 123.74      | 121.00   |
| 51  | A2    | 959  | C    | C2-N1-C1'  | -5.47 | 112.78      | 118.80   |
| 51  | A2    | 3679 | C    | C5-C6-N1   | 5.47  | 123.74      | 121.00   |
| 51  | A2    | 4327 | C    | C5-C6-N1   | 5.47  | 123.74      | 121.00   |
| 52  | B1    | 1517 | G    | C2-N3-C4   | -5.47 | 109.16      | 111.90   |
| 52  | B1    | 1441 | U    | C2-N1-C1'  | 5.47  | 124.27      | 117.70   |
| 51  | A2    | 4644 | U    | N3-C2-O2   | -5.47 | 118.37      | 122.20   |
| 51  | A2    | 4906 | C    | C6-N1-C2   | -5.47 | 118.11      | 120.30   |
| 51  | A2    | 1966 | G    | N3-C4-N9   | 5.47  | 129.28      | 126.00   |
| 8   | A4    | 14   | C    | C6-N1-C1'  | -5.47 | 114.24      | 120.80   |
| 52  | B1    | 4    | C    | C6-N1-C2   | -5.47 | 118.11      | 120.30   |
| 52  | B1    | 1600 | G    | N3-C4-N9   | 5.47  | 129.28      | 126.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 52  | B1    | 879  | C    | C2-N1-C1'   | 5.46  | 124.81      | 118.80   |
| 52  | B1    | 942  | G    | C4-N9-C1'   | 5.46  | 133.59      | 126.50   |
| 52  | B1    | 100  | U    | N3-C2-O2    | -5.45 | 118.38      | 122.20   |
| 28  | AW    | 59   | HIS  | C-N-CA      | 5.45  | 135.33      | 121.70   |
| 51  | A2    | 504  | U    | N3-C2-O2    | -5.45 | 118.38      | 122.20   |
| 51  | A2    | 4431 | U    | N3-C2-O2    | -5.45 | 118.39      | 122.20   |
| 51  | A2    | 4602 | C    | C6-N1-C1'   | -5.45 | 114.26      | 120.80   |
| 51  | A2    | 2611 | U    | N3-C2-O2    | -5.45 | 118.39      | 122.20   |
| 51  | A2    | 727  | C    | C6-N1-C2    | -5.44 | 118.12      | 120.30   |
| 52  | B1    | 220  | U    | N3-C2-O2    | -5.44 | 118.39      | 122.20   |
| 52  | B1    | 174  | C    | N1-C2-O2    | 5.44  | 122.17      | 118.90   |
| 51  | A2    | 962  | C    | N3-C2-O2    | -5.44 | 118.09      | 121.90   |
| 51  | A2    | 1638 | U    | C2-N1-C1'   | 5.44  | 124.23      | 117.70   |
| 51  | A2    | 3737 | A    | O4'-C1'-N9  | 5.44  | 112.55      | 108.20   |
| 51  | A2    | 4423 | C    | C6-N1-C2    | -5.44 | 118.12      | 120.30   |
| 51  | A2    | 509  | C    | C5-C6-N1    | 5.44  | 123.72      | 121.00   |
| 51  | A2    | 4523 | C    | C2-N1-C1'   | 5.44  | 124.78      | 118.80   |
| 51  | A2    | 1737 | C    | C6-N1-C2    | -5.43 | 118.13      | 120.30   |
| 52  | B1    | 534  | G    | N7-C8-N9    | 5.43  | 115.82      | 113.10   |
| 51  | A2    | 3890 | C    | C5-C6-N1    | 5.43  | 123.72      | 121.00   |
| 51  | A2    | 4853 | C    | C6-N1-C2    | -5.43 | 118.13      | 120.30   |
| 51  | A2    | 185  | G    | C4-N9-C1'   | 5.43  | 133.56      | 126.50   |
| 52  | B1    | 645  | C    | C5-C6-N1    | 5.43  | 123.71      | 121.00   |
| 51  | A2    | 275  | U    | N3-C2-O2    | -5.43 | 118.40      | 122.20   |
| 51  | A2    | 4151 | U    | C2-N1-C1'   | 5.43  | 124.21      | 117.70   |
| 52  | B1    | 1163 | C    | C2-N1-C1'   | 5.42  | 124.77      | 118.80   |
| 51  | A2    | 4333 | G    | P-O3'-C3'   | 5.42  | 126.21      | 119.70   |
| 51  | A2    | 1707 | U    | N3-C2-O2    | -5.42 | 118.41      | 122.20   |
| 51  | A2    | 2606 | C    | N3-C2-O2    | -5.42 | 118.11      | 121.90   |
| 51  | A2    | 175  | C    | N3-C2-O2    | -5.42 | 118.11      | 121.90   |
| 52  | B1    | 1314 | U    | N3-C2-O2    | -5.42 | 118.41      | 122.20   |
| 51  | A2    | 2805 | U    | N3-C2-O2    | -5.42 | 118.41      | 122.20   |
| 52  | B1    | 295  | C    | C6-N1-C2    | -5.41 | 118.13      | 120.30   |
| 51  | A2    | 4103 | C    | N1-C2-O2    | 5.41  | 122.15      | 118.90   |
| 52  | B1    | 173  | A    | C3'-C2'-C1' | 5.41  | 105.83      | 101.50   |
| 51  | A2    | 3738 | C    | N1-C2-O2    | 5.41  | 122.14      | 118.90   |
| 51  | A2    | 645  | C    | C6-N1-C1'   | -5.41 | 114.31      | 120.80   |
| 51  | A2    | 1708 | U    | N3-C2-O2    | -5.41 | 118.42      | 122.20   |
| 52  | B1    | 1464 | C    | C6-N1-C2    | -5.41 | 118.14      | 120.30   |
| 51  | A2    | 258  | C    | N1-C2-O2    | 5.40  | 122.14      | 118.90   |
| 51  | A2    | 1722 | C    | N1-C2-O2    | 5.40  | 122.14      | 118.90   |
| 51  | A2    | 3638 | C    | C6-N1-C2    | -5.40 | 118.14      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 51  | A2    | 4085 | C    | N1-C2-O2  | 5.40  | 122.14      | 118.90   |
| 52  | B1    | 44   | U    | N3-C2-O2  | -5.40 | 118.42      | 122.20   |
| 51  | A2    | 671  | C    | C6-N1-C2  | -5.40 | 118.14      | 120.30   |
| 7   | A3    | 99   | U    | N1-C2-O2  | 5.40  | 126.58      | 122.80   |
| 51  | A2    | 1163 | C    | N1-C2-O2  | 5.40  | 122.14      | 118.90   |
| 51  | A2    | 4388 | C    | C6-N1-C2  | -5.40 | 118.14      | 120.30   |
| 51  | A2    | 2793 | C    | N1-C2-O2  | 5.39  | 122.14      | 118.90   |
| 52  | B1    | 537  | C    | C6-N1-C2  | -5.39 | 118.14      | 120.30   |
| 51  | A2    | 911  | C    | N1-C2-O2  | 5.39  | 122.13      | 118.90   |
| 51  | A2    | 2649 | C    | C2-N1-C1' | 5.39  | 124.73      | 118.80   |
| 61  | BL    | 42   | LEU  | CA-CB-CG  | 5.39  | 127.69      | 115.30   |
| 52  | B1    | 498  | C    | C5-C6-N1  | 5.39  | 123.69      | 121.00   |
| 52  | B1    | 942  | G    | C8-N9-C4  | -5.39 | 104.25      | 106.40   |
| 51  | A2    | 4731 | G    | C4-N9-C1' | 5.38  | 133.50      | 126.50   |
| 52  | B1    | 1624 | U    | C5-C6-N1  | 5.38  | 125.39      | 122.70   |
| 39  | Ah    | 28   | LEU  | CA-CB-CG  | 5.38  | 127.68      | 115.30   |
| 51  | A2    | 2871 | C    | C6-N1-C2  | -5.38 | 118.15      | 120.30   |
| 51  | A2    | 4728 | C    | N1-C2-O2  | 5.38  | 122.13      | 118.90   |
| 52  | B1    | 1117 | C    | N3-C2-O2  | -5.38 | 118.14      | 121.90   |
| 52  | B1    | 1315 | U    | C6-N1-C2  | -5.38 | 117.77      | 121.00   |
| 51  | A2    | 2817 | G    | C4-N9-C1' | 5.37  | 133.49      | 126.50   |
| 7   | A3    | 108  | A    | P-O3'-C3' | 5.37  | 126.14      | 119.70   |
| 51  | A2    | 2308 | U    | C2-N1-C1' | 5.37  | 124.14      | 117.70   |
| 51  | A2    | 2308 | U    | N1-C2-O2  | 5.37  | 126.56      | 122.80   |
| 51  | A2    | 4602 | C    | C5-C6-N1  | 5.37  | 123.68      | 121.00   |
| 52  | B1    | 1441 | U    | N1-C2-O2  | 5.37  | 126.56      | 122.80   |
| 51  | A2    | 175  | C    | N1-C2-O2  | 5.36  | 122.12      | 118.90   |
| 51  | A2    | 1059 | C    | C5-C6-N1  | 5.36  | 123.68      | 121.00   |
| 51  | A2    | 1794 | C    | C6-N1-C2  | -5.36 | 118.16      | 120.30   |
| 51  | A2    | 4072 | C    | C5-C6-N1  | 5.36  | 123.68      | 121.00   |
| 52  | B1    | 1120 | U    | C2-N1-C1' | 5.36  | 124.13      | 117.70   |
| 51  | A2    | 492  | C    | O5'-P-OP1 | 5.36  | 117.13      | 110.70   |
| 51  | A2    | 4177 | C    | N1-C2-O2  | 5.36  | 122.11      | 118.90   |
| 51  | A2    | 2835 | C    | N3-C2-O2  | -5.36 | 118.15      | 121.90   |
| 51  | A2    | 4191 | U    | N1-C2-O2  | 5.36  | 126.55      | 122.80   |
| 51  | A2    | 2373 | G    | N3-C4-N9  | 5.35  | 129.21      | 126.00   |
| 51  | A2    | 4602 | C    | C6-N1-C2  | -5.35 | 118.16      | 120.30   |
| 52  | B1    | 1130 | G    | N3-C4-N9  | -5.35 | 122.79      | 126.00   |
| 52  | B1    | 1811 | C    | C6-N1-C2  | -5.35 | 118.16      | 120.30   |
| 69  | BT    | 64   | LEU  | CA-CB-CG  | 5.35  | 127.61      | 115.30   |
| 51  | A2    | 2325 | C    | N3-C2-O2  | -5.35 | 118.15      | 121.90   |
| 52  | B1    | 1512 | C    | N1-C2-O2  | 5.35  | 122.11      | 118.90   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 52  | B1    | 1123 | C    | C5-C6-N1  | 5.35  | 123.67      | 121.00   |
| 51  | A2    | 644  | C    | C6-N1-C2  | -5.34 | 118.16      | 120.30   |
| 52  | B1    | 1591 | C    | N3-C2-O2  | -5.34 | 118.16      | 121.90   |
| 52  | B1    | 1292 | C    | N3-C2-O2  | -5.34 | 118.16      | 121.90   |
| 51  | A2    | 3864 | C    | C5-C6-N1  | 5.33  | 123.67      | 121.00   |
| 51  | A2    | 898  | U    | N3-C2-O2  | -5.33 | 118.47      | 122.20   |
| 51  | A2    | 2330 | C    | C6-N1-C1' | -5.33 | 114.40      | 120.80   |
| 52  | B1    | 950  | C    | C5-C6-N1  | 5.33  | 123.67      | 121.00   |
| 51  | A2    | 4103 | C    | C5-C6-N1  | 5.33  | 123.67      | 121.00   |
| 51  | A2    | 3824 | U    | C2-N1-C1' | 5.33  | 124.09      | 117.70   |
| 51  | A2    | 513  | C    | N1-C2-O2  | 5.32  | 122.09      | 118.90   |
| 51  | A2    | 214  | C    | C2-N1-C1' | 5.32  | 124.65      | 118.80   |
| 8   | A4    | 19   | C    | C6-N1-C2  | -5.32 | 118.17      | 120.30   |
| 52  | B1    | 1032 | C    | C5-C6-N1  | 5.32  | 123.66      | 121.00   |
| 51  | A2    | 1995 | C    | N3-C2-O2  | -5.32 | 118.18      | 121.90   |
| 51  | A2    | 2282 | C    | C5-C6-N1  | 5.32  | 123.66      | 121.00   |
| 51  | A2    | 4880 | C    | C6-N1-C1' | -5.32 | 114.42      | 120.80   |
| 52  | B1    | 695  | C    | N1-C2-O2  | 5.32  | 122.09      | 118.90   |
| 51  | A2    | 1930 | U    | N1-C2-O2  | 5.31  | 126.52      | 122.80   |
| 51  | A2    | 2547 | C    | C6-N1-C2  | -5.31 | 118.18      | 120.30   |
| 50  | Au    | 29   | LEU  | CA-CB-CG  | 5.31  | 127.51      | 115.30   |
| 79  | Bd    | 39   | CYS  | C-N-CA    | 5.30  | 134.96      | 121.70   |
| 51  | A2    | 1607 | G    | C8-N9-C1' | -5.30 | 120.11      | 127.00   |
| 52  | B1    | 293  | C    | N3-C4-N4  | 5.30  | 121.71      | 118.00   |
| 51  | A2    | 4575 | C    | N1-C2-O2  | 5.29  | 122.08      | 118.90   |
| 51  | A2    | 1794 | C    | C2-N1-C1' | 5.29  | 124.62      | 118.80   |
| 51  | A2    | 3725 | G    | C8-N9-C1' | 5.29  | 133.88      | 127.00   |
| 52  | B1    | 233  | C    | N1-C2-O2  | 5.29  | 122.08      | 118.90   |
| 52  | B1    | 1186 | U    | N3-C2-O2  | -5.29 | 118.50      | 122.20   |
| 52  | B1    | 1314 | U    | N1-C2-O2  | 5.29  | 126.50      | 122.80   |
| 83  | Bv    | 43   | C    | N3-C2-O2  | -5.29 | 118.20      | 121.90   |
| 51  | A2    | 918  | C    | C6-N1-C1' | -5.28 | 114.46      | 120.80   |
| 51  | A2    | 2330 | C    | C5-C6-N1  | 5.28  | 123.64      | 121.00   |
| 51  | A2    | 2606 | C    | C6-N1-C2  | -5.28 | 118.19      | 120.30   |
| 51  | A2    | 1256 | G    | C8-N9-C1' | -5.27 | 120.14      | 127.00   |
| 7   | A3    | 116  | C    | C2-N1-C1' | 5.27  | 124.59      | 118.80   |
| 51  | A2    | 4979 | C    | C6-N1-C2  | -5.27 | 118.19      | 120.30   |
| 52  | B1    | 53   | C    | C2-N1-C1' | 5.27  | 124.59      | 118.80   |
| 52  | B1    | 552  | G    | N7-C8-N9  | 5.27  | 115.73      | 113.10   |
| 52  | B1    | 960  | U    | N3-C2-O2  | -5.26 | 118.52      | 122.20   |
| 7   | A3    | 116  | C    | C6-N1-C2  | -5.26 | 118.19      | 120.30   |
| 51  | A2    | 4010 | C    | C2-N1-C1' | 5.26  | 124.59      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 51  | A2    | 1607 | G    | N3-C4-N9   | 5.26  | 129.16      | 126.00   |
| 51  | A2    | 191  | C    | N3-C2-O2   | -5.25 | 118.22      | 121.90   |
| 52  | B1    | 106  | C    | C6-N1-C2   | -5.25 | 118.20      | 120.30   |
| 28  | AW    | 82   | ILE  | CG1-CB-CG2 | -5.25 | 99.84       | 111.40   |
| 51  | A2    | 1268 | U    | C5-C6-N1   | -5.25 | 120.07      | 122.70   |
| 51  | A2    | 2400 | G    | N3-C4-N9   | 5.25  | 129.15      | 126.00   |
| 11  | AF    | 165  | LYS  | CA-CB-CG   | 5.25  | 124.95      | 113.40   |
| 51  | A2    | 96   | U    | N3-C2-O2   | -5.25 | 118.53      | 122.20   |
| 52  | B1    | 1352 | G    | C4-N9-C1'  | 5.25  | 133.32      | 126.50   |
| 51  | A2    | 251  | G    | C2-N3-C4   | 5.25  | 114.52      | 111.90   |
| 51  | A2    | 1745 | C    | C6-N1-C2   | -5.25 | 118.20      | 120.30   |
| 51  | A2    | 1975 | C    | N1-C2-O2   | 5.25  | 122.05      | 118.90   |
| 51  | A2    | 217  | C    | C6-N1-C2   | -5.25 | 118.20      | 120.30   |
| 52  | B1    | 179  | C    | C2-N1-C1'  | 5.25  | 124.57      | 118.80   |
| 7   | A3    | 57   | C    | N1-C2-O2   | 5.24  | 122.04      | 118.90   |
| 51  | A2    | 962  | C    | C6-N1-C2   | -5.24 | 118.20      | 120.30   |
| 51  | A2    | 2766 | A    | C4-N9-C1'  | 5.24  | 135.73      | 126.30   |
| 52  | B1    | 559  | G    | N3-C4-N9   | -5.24 | 122.86      | 126.00   |
| 51  | A2    | 78   | U    | N3-C2-O2   | -5.24 | 118.53      | 122.20   |
| 52  | B1    | 645  | C    | C6-N1-C2   | -5.24 | 118.21      | 120.30   |
| 51  | A2    | 701  | G    | C8-N9-C4   | -5.23 | 104.31      | 106.40   |
| 51  | A2    | 493  | G    | N3-C4-C5   | -5.23 | 125.98      | 128.60   |
| 12  | AG    | 83   | PHE  | C-N-CA     | 5.23  | 134.77      | 121.70   |
| 51  | A2    | 4993 | U    | N3-C2-O2   | -5.23 | 118.54      | 122.20   |
| 51  | A2    | 1596 | C    | C2-N1-C1'  | 5.23  | 124.55      | 118.80   |
| 51  | A2    | 4302 | U    | N1-C2-O2   | 5.23  | 126.46      | 122.80   |
| 52  | B1    | 567  | C    | N1-C2-O2   | 5.23  | 122.04      | 118.90   |
| 51  | A2    | 1947 | C    | C5-C6-N1   | 5.23  | 123.61      | 121.00   |
| 51  | A2    | 1163 | C    | C2-N1-C1'  | 5.22  | 124.55      | 118.80   |
| 52  | B1    | 1053 | C    | C5-C6-N1   | 5.22  | 123.61      | 121.00   |
| 52  | B1    | 178  | C    | N3-C2-O2   | -5.22 | 118.25      | 121.90   |
| 51  | A2    | 2330 | C    | N1-C2-O2   | 5.22  | 122.03      | 118.90   |
| 52  | B1    | 579  | C    | N1-C2-O2   | 5.22  | 122.03      | 118.90   |
| 52  | B1    | 1022 | U    | C2-N1-C1'  | 5.22  | 123.96      | 117.70   |
| 51  | A2    | 167  | C    | N1-C2-O2   | 5.21  | 122.03      | 118.90   |
| 51  | A2    | 3628 | U    | N3-C2-O2   | -5.20 | 118.56      | 122.20   |
| 51  | A2    | 1082 | C    | N3-C2-O2   | -5.20 | 118.26      | 121.90   |
| 51  | A2    | 1704 | C    | C6-N1-C2   | -5.20 | 118.22      | 120.30   |
| 51  | A2    | 2042 | U    | N3-C2-O2   | -5.20 | 118.56      | 122.20   |
| 51  | A2    | 3679 | C    | C6-N1-C2   | -5.20 | 118.22      | 120.30   |
| 51  | A2    | 4071 | C    | N1-C2-O2   | 5.20  | 122.02      | 118.90   |
| 51  | A2    | 4302 | U    | N3-C2-O2   | -5.20 | 118.56      | 122.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 52  | B1    | 796  | G    | N3-C4-N9   | 5.20  | 129.12      | 126.00   |
| 51  | A2    | 167  | C    | N3-C2-O2   | -5.19 | 118.27      | 121.90   |
| 51  | A2    | 163  | C    | C6-N1-C2   | -5.19 | 118.22      | 120.30   |
| 51  | A2    | 2457 | C    | C6-N1-C2   | -5.19 | 118.22      | 120.30   |
| 51  | A2    | 962  | C    | C2-N1-C1'  | 5.19  | 124.51      | 118.80   |
| 52  | B1    | 325  | C    | C6-N1-C2   | -5.19 | 118.22      | 120.30   |
| 48  | Aq    | 35   | LEU  | CA-CB-CG   | 5.19  | 127.23      | 115.30   |
| 51  | A2    | 637  | C    | N3-C2-O2   | -5.19 | 118.27      | 121.90   |
| 51  | A2    | 3742 | C    | N1-C2-O2   | -5.19 | 115.79      | 118.90   |
| 51  | A2    | 4105 | C    | C6-N1-C2   | -5.19 | 118.22      | 120.30   |
| 52  | B1    | 1590 | C    | N1-C2-O2   | 5.19  | 122.01      | 118.90   |
| 52  | B1    | 1482 | C    | C6-N1-C2   | -5.18 | 118.23      | 120.30   |
| 22  | AQ    | 63   | LEU  | CA-CB-CG   | 5.18  | 127.22      | 115.30   |
| 51  | A2    | 2662 | C    | C6-N1-C2   | -5.18 | 118.23      | 120.30   |
| 52  | B1    | 1554 | C    | N1-C2-O2   | 5.18  | 122.01      | 118.90   |
| 51  | A2    | 4135 | G    | C4-N9-C1'  | 5.18  | 133.24      | 126.50   |
| 52  | B1    | 534  | G    | C6-C5-N7   | -5.18 | 127.29      | 130.40   |
| 51  | A2    | 4661 | U    | P-O3'-C3'  | 5.18  | 125.92      | 119.70   |
| 52  | B1    | 534  | G    | N3-C4-N9   | 5.18  | 129.11      | 126.00   |
| 52  | B1    | 960  | U    | N1-C2-O2   | 5.18  | 126.43      | 122.80   |
| 51  | A2    | 2646 | C    | C6-N1-C2   | -5.18 | 118.23      | 120.30   |
| 39  | Ah    | 47   | ILE  | CG1-CB-CG2 | -5.18 | 100.01      | 111.40   |
| 51  | A2    | 4177 | C    | N3-C2-O2   | -5.18 | 118.28      | 121.90   |
| 83  | Bv    | 20   | U    | C5-C6-N1   | 5.17  | 125.29      | 122.70   |
| 51  | A2    | 669  | G    | N1-C2-N3   | 5.17  | 127.00      | 123.90   |
| 51  | A2    | 2829 | A    | C4-N9-C1'  | 5.16  | 135.59      | 126.30   |
| 51  | A2    | 1401 | C    | C6-N1-C2   | -5.16 | 118.24      | 120.30   |
| 51  | A2    | 3661 | U    | N3-C2-O2   | -5.16 | 118.59      | 122.20   |
| 52  | B1    | 233  | C    | C2-N1-C1'  | 5.16  | 124.48      | 118.80   |
| 51  | A2    | 1914 | G    | N7-C8-N9   | 5.16  | 115.68      | 113.10   |
| 51  | A2    | 2511 | C    | N1-C2-O2   | 5.16  | 121.99      | 118.90   |
| 52  | B1    | 120  | U    | N3-C2-O2   | -5.16 | 118.59      | 122.20   |
| 52  | B1    | 1862 | G    | OP1-P-O3'  | 5.16  | 116.55      | 105.20   |
| 13  | AH    | 142  | ASP  | CB-CG-OD1  | 5.15  | 122.94      | 118.30   |
| 51  | A2    | 4177 | C    | C6-N1-C2   | -5.15 | 118.24      | 120.30   |
| 52  | B1    | 1135 | C    | C5-C6-N1   | 5.15  | 123.58      | 121.00   |
| 52  | B1    | 1425 | G    | N3-C4-C5   | -5.15 | 126.02      | 128.60   |
| 51  | A2    | 1773 | U    | N1-C2-O2   | 5.15  | 126.40      | 122.80   |
| 52  | B1    | 682  | U    | N3-C2-O2   | -5.15 | 118.60      | 122.20   |
| 51  | A2    | 674  | C    | C2-N1-C1'  | 5.14  | 124.46      | 118.80   |
| 51  | A2    | 4048 | C    | C6-N1-C2   | -5.14 | 118.24      | 120.30   |
| 52  | B1    | 745  | C    | C2-N1-C1'  | 5.14  | 124.46      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 51  | A2    | 2418 | G    | N3-C4-C5   | -5.14 | 126.03      | 128.60   |
| 52  | B1    | 293  | C    | C5-C4-N4   | -5.14 | 116.60      | 120.20   |
| 51  | A2    | 2691 | G    | C4-N9-C1'  | 5.14  | 133.18      | 126.50   |
| 51  | A2    | 498  | G    | N7-C8-N9   | 5.14  | 115.67      | 113.10   |
| 51  | A2    | 444  | G    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 51  | A2    | 2646 | C    | C2-N1-C1'  | 5.14  | 124.45      | 118.80   |
| 51  | A2    | 4088 | C    | C5-C6-N1   | 5.13  | 123.57      | 121.00   |
| 52  | B1    | 298  | G    | C8-N9-C1'  | -5.13 | 120.33      | 127.00   |
| 52  | B1    | 1750 | C    | N1-C2-O2   | 5.13  | 121.98      | 118.90   |
| 51  | A2    | 669  | G    | N3-C2-N2   | -5.13 | 116.31      | 119.90   |
| 52  | B1    | 233  | C    | C6-N1-C2   | -5.12 | 118.25      | 120.30   |
| 42  | Ak    | 60   | LEU  | CA-CB-CG   | 5.12  | 127.08      | 115.30   |
| 51  | A2    | 2799 | C    | C6-N1-C2   | -5.12 | 118.25      | 120.30   |
| 52  | B1    | 1517 | G    | N3-C2-N2   | -5.12 | 116.31      | 119.90   |
| 52  | B1    | 459  | C    | C6-N1-C2   | -5.12 | 118.25      | 120.30   |
| 51  | A2    | 6    | C    | C6-N1-C2   | -5.12 | 118.25      | 120.30   |
| 7   | A3    | 96   | C    | C2-N1-C1'  | 5.12  | 124.43      | 118.80   |
| 51  | A2    | 4930 | U    | N3-C2-O2   | -5.12 | 118.62      | 122.20   |
| 51  | A2    | 14   | C    | C6-N1-C2   | -5.11 | 118.26      | 120.30   |
| 51  | A2    | 648  | C    | O4'-C1'-N1 | 5.11  | 112.29      | 108.20   |
| 51  | A2    | 2706 | C    | C5-C6-N1   | 5.11  | 123.55      | 121.00   |
| 51  | A2    | 3927 | G    | N3-C4-N9   | -5.11 | 122.94      | 126.00   |
| 52  | B1    | 942  | G    | N3-C4-C5   | -5.10 | 126.05      | 128.60   |
| 51  | A2    | 4133 | C    | N1-C2-O2   | 5.10  | 121.96      | 118.90   |
| 52  | B1    | 578  | C    | N3-C2-O2   | -5.10 | 118.33      | 121.90   |
| 51  | A2    | 2706 | C    | C2-N1-C1'  | 5.10  | 124.41      | 118.80   |
| 52  | B1    | 1520 | G    | N7-C8-N9   | 5.09  | 115.65      | 113.10   |
| 51  | A2    | 1594 | G    | C4-N9-C1'  | 5.09  | 133.12      | 126.50   |
| 52  | B1    | 537  | C    | C5-C6-N1   | 5.09  | 123.55      | 121.00   |
| 52  | B1    | 1117 | C    | C5-C6-N1   | 5.09  | 123.55      | 121.00   |
| 51  | A2    | 1763 | U    | N3-C2-O2   | -5.09 | 118.64      | 122.20   |
| 51  | A2    | 4574 | C    | N1-C2-O2   | 5.09  | 121.95      | 118.90   |
| 51  | A2    | 2706 | C    | N1-C2-O2   | 5.09  | 121.95      | 118.90   |
| 51  | A2    | 2879 | U    | C2-N1-C1'  | 5.09  | 123.80      | 117.70   |
| 51  | A2    | 3725 | G    | C6-C5-N7   | 5.08  | 133.45      | 130.40   |
| 51  | A2    | 4624 | C    | C2-N1-C1'  | 5.08  | 124.39      | 118.80   |
| 51  | A2    | 4538 | U    | C2-N1-C1'  | 5.08  | 123.80      | 117.70   |
| 52  | B1    | 100  | U    | C2-N1-C1'  | 5.08  | 123.80      | 117.70   |
| 52  | B1    | 1591 | C    | C2-N1-C1'  | 5.08  | 124.39      | 118.80   |
| 51  | A2    | 1947 | C    | N1-C2-O2   | 5.08  | 121.95      | 118.90   |
| 52  | B1    | 577  | U    | N3-C2-O2   | -5.08 | 118.65      | 122.20   |
| 52  | B1    | 494  | C    | N1-C2-O2   | 5.07  | 121.94      | 118.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 51  | A2    | 1952 | C    | N1-C2-O2   | 5.07  | 121.94      | 118.90   |
| 51  | A2    | 4489 | G    | C6-C5-N7   | -5.07 | 127.36      | 130.40   |
| 51  | A2    | 1267 | G    | C4-N9-C1'  | 5.07  | 133.09      | 126.50   |
| 52  | B1    | 189  | U    | N3-C2-O2   | -5.07 | 118.65      | 122.20   |
| 8   | A4    | 47   | G    | C4-C5-N7   | 5.06  | 112.83      | 110.80   |
| 52  | B1    | 1558 | C    | C6-N1-C2   | -5.06 | 118.28      | 120.30   |
| 52  | B1    | 1622 | U    | C2-N1-C1'  | 5.06  | 123.77      | 117.70   |
| 51  | A2    | 4880 | C    | O4'-C1'-N1 | 5.06  | 112.25      | 108.20   |
| 52  | B1    | 1441 | U    | N3-C2-O2   | -5.06 | 118.66      | 122.20   |
| 52  | B1    | 1586 | U    | C6-N1-C1'  | -5.06 | 114.12      | 121.20   |
| 51  | A2    | 74   | G    | C4-N9-C1'  | 5.06  | 133.07      | 126.50   |
| 51  | A2    | 4824 | C    | C2-N1-C1'  | 5.06  | 124.36      | 118.80   |
| 51  | A2    | 4589 | U    | N3-C2-O2   | -5.06 | 118.66      | 122.20   |
| 51  | A2    | 1284 | C    | C6-N1-C1'  | 5.05  | 126.86      | 120.80   |
| 34  | Ac    | 45   | LEU  | CA-CB-CG   | 5.05  | 126.92      | 115.30   |
| 52  | B1    | 1203 | G    | C4-N9-C1'  | 5.05  | 133.07      | 126.50   |
| 51  | A2    | 1737 | C    | C5-C6-N1   | 5.05  | 123.53      | 121.00   |
| 51  | A2    | 4856 | G    | C4-N9-C1'  | 5.05  | 133.06      | 126.50   |
| 51  | A2    | 4066 | C    | N1-C2-O2   | 5.05  | 121.93      | 118.90   |
| 52  | B1    | 325  | C    | N3-C2-O2   | -5.05 | 118.37      | 121.90   |
| 52  | B1    | 1163 | C    | N3-C2-O2   | -5.05 | 118.37      | 121.90   |
| 52  | B1    | 1690 | U    | N1-C2-O2   | 5.05  | 126.33      | 122.80   |
| 51  | A2    | 515  | C    | N1-C2-O2   | 5.04  | 121.93      | 118.90   |
| 51  | A2    | 2805 | U    | N1-C2-O2   | 5.04  | 126.33      | 122.80   |
| 51  | A2    | 478  | U    | C5-C6-N1   | 5.04  | 125.22      | 122.70   |
| 51  | A2    | 668  | C    | N1-C2-O2   | 5.04  | 121.92      | 118.90   |
| 51  | A2    | 4878 | C    | N3-C2-O2   | -5.04 | 118.37      | 121.90   |
| 52  | B1    | 192  | C    | N1-C2-O2   | 5.04  | 121.92      | 118.90   |
| 51  | A2    | 48   | G    | C4-N9-C1'  | -5.04 | 119.95      | 126.50   |
| 51  | A2    | 480  | C    | C5-C6-N1   | 5.04  | 123.52      | 121.00   |
| 51  | A2    | 1058 | G    | C8-N9-C4   | -5.04 | 104.39      | 106.40   |
| 51  | A2    | 4482 | G    | C4-N9-C1'  | 5.04  | 133.05      | 126.50   |
| 51  | A2    | 3822 | U    | C2-N1-C1'  | 5.03  | 123.74      | 117.70   |
| 51  | A2    | 4161 | C    | N1-C2-O2   | 5.03  | 121.92      | 118.90   |
| 52  | B1    | 1520 | G    | C2-N3-C4   | 5.03  | 114.42      | 111.90   |
| 52  | B1    | 1123 | C    | N1-C2-O2   | 5.03  | 121.92      | 118.90   |
| 51  | A2    | 637  | C    | C6-N1-C2   | -5.03 | 118.29      | 120.30   |
| 51  | A2    | 1269 | C    | O4'-C1'-N1 | 5.03  | 112.22      | 108.20   |
| 51  | A2    | 197  | U    | C6-N1-C2   | -5.03 | 117.98      | 121.00   |
| 51  | A2    | 1914 | G    | C6-C5-N7   | -5.02 | 127.39      | 130.40   |
| 51  | A2    | 1450 | C    | C6-N1-C2   | -5.02 | 118.29      | 120.30   |
| 51  | A2    | 959  | C    | C6-N1-C1'  | 5.02  | 126.82      | 120.80   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 51  | A2    | 960  | G    | N7-C8-N9  | 5.01  | 115.61      | 113.10   |
| 51  | A2    | 1653 | U    | C2-N1-C1' | 5.01  | 123.72      | 117.70   |
| 51  | A2    | 2256 | C    | C5-C6-N1  | 5.01  | 123.51      | 121.00   |
| 51  | A2    | 652  | C    | C6-N1-C2  | -5.01 | 118.30      | 120.30   |
| 51  | A2    | 2706 | C    | C6-N1-C2  | -5.01 | 118.30      | 120.30   |
| 51  | A2    | 1082 | C    | N1-C2-O2  | 5.01  | 121.91      | 118.90   |
| 52  | B1    | 927  | C    | N3-C2-O2  | -5.01 | 118.39      | 121.90   |
| 52  | B1    | 4    | C    | C5-C6-N1  | 5.01  | 123.50      | 121.00   |
| 51  | A2    | 1065 | C    | N1-C2-O2  | 5.01  | 121.90      | 118.90   |
| 51  | A2    | 2592 | C    | N3-C2-O2  | -5.00 | 118.40      | 121.90   |
| 52  | B1    | 796  | G    | N3-C4-C5  | -5.00 | 126.10      | 128.60   |
| 52  | B1    | 1517 | G    | N3-C4-C5  | 5.00  | 131.10      | 128.60   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 9   | AD    | 228 | LYS  | Peptide |
| 13  | AH    | 116 | ASN  | Peptide |
| 29  | AX    | 79  | PHE  | Peptide |
| 4   | BB    | 39  | PHE  | 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 |
|-----|-------|---------------|-----------|----------|----------|-------------|
| 1   | AA    | 250/257 (97%) | 223 (89%) | 24 (10%) | 3 (1%)   | 13 41       |
| 2   | BA    | 213/215 (99%) | 196 (92%) | 13 (6%)  | 4 (2%)   | 8 31        |

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| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 3   | AB    | 392/394 (100%) | 363 (93%) | 29 (7%)  | 0        | 100         | 100 |
| 4   | BB    | 210/212 (99%)  | 181 (86%) | 27 (13%) | 2 (1%)   | 15          | 46  |
| 5   | AC    | 361/363 (99%)  | 333 (92%) | 26 (7%)  | 2 (1%)   | 25          | 57  |
| 6   | BC    | 220/222 (99%)  | 205 (93%) | 15 (7%)  | 0        | 100         | 100 |
| 9   | AD    | 292/294 (99%)  | 261 (89%) | 27 (9%)  | 4 (1%)   | 11          | 37  |
| 10  | AE    | 192/194 (99%)  | 159 (83%) | 29 (15%) | 4 (2%)   | 7           | 30  |
| 11  | AF    | 232/234 (99%)  | 211 (91%) | 20 (9%)  | 1 (0%)   | 34          | 67  |
| 12  | AG    | 232/234 (99%)  | 211 (91%) | 21 (9%)  | 0        | 100         | 100 |
| 13  | AH    | 189/191 (99%)  | 178 (94%) | 9 (5%)   | 2 (1%)   | 14          | 44  |
| 14  | AI    | 204/211 (97%)  | 182 (89%) | 22 (11%) | 0        | 100         | 100 |
| 15  | AJ    | 167/169 (99%)  | 153 (92%) | 12 (7%)  | 2 (1%)   | 13          | 41  |
| 16  | AK    | 107/109 (98%)  | 59 (55%)  | 35 (33%) | 13 (12%) | 0           | 2   |
| 17  | AL    | 203/205 (99%)  | 166 (82%) | 28 (14%) | 9 (4%)   | 2           | 16  |
| 18  | AM    | 137/139 (99%)  | 125 (91%) | 12 (9%)  | 0        | 100         | 100 |
| 19  | AN    | 201/203 (99%)  | 184 (92%) | 16 (8%)  | 1 (0%)   | 29          | 61  |
| 20  | AO    | 193/195 (99%)  | 180 (93%) | 13 (7%)  | 0        | 100         | 100 |
| 21  | AP    | 151/153 (99%)  | 147 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 22  | AQ    | 185/187 (99%)  | 159 (86%) | 25 (14%) | 1 (0%)   | 29          | 61  |
| 23  | AR    | 179/181 (99%)  | 169 (94%) | 9 (5%)   | 1 (1%)   | 25          | 57  |
| 24  | AS    | 173/175 (99%)  | 162 (94%) | 11 (6%)  | 0        | 100         | 100 |
| 25  | AT    | 155/157 (99%)  | 140 (90%) | 13 (8%)  | 2 (1%)   | 12          | 39  |
| 26  | AU    | 97/99 (98%)    | 87 (90%)  | 8 (8%)   | 2 (2%)   | 7           | 30  |
| 27  | AV    | 127/129 (98%)  | 122 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 28  | AW    | 119/121 (98%)  | 105 (88%) | 13 (11%) | 1 (1%)   | 19          | 51  |
| 29  | AX    | 115/117 (98%)  | 110 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 30  | AY    | 125/127 (98%)  | 118 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 31  | AZ    | 132/134 (98%)  | 117 (89%) | 15 (11%) | 0        | 100         | 100 |
| 32  | Aa    | 145/147 (99%)  | 128 (88%) | 17 (12%) | 0        | 100         | 100 |
| 33  | Ab    | 66/121 (54%)   | 56 (85%)  | 9 (14%)  | 1 (2%)   | 10          | 36  |
| 34  | Ac    | 101/103 (98%)  | 96 (95%)  | 3 (3%)   | 2 (2%)   | 7           | 30  |
| 35  | Ad    | 104/106 (98%)  | 99 (95%)  | 5 (5%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 36  | Ae    | 127/129 (98%) | 113 (89%) | 14 (11%) | 0        | 100         | 100 |
| 37  | Af    | 107/109 (98%) | 95 (89%)  | 9 (8%)   | 3 (3%)   | 5           | 24  |
| 38  | Ag    | 112/114 (98%) | 101 (90%) | 11 (10%) | 0        | 100         | 100 |
| 39  | Ah    | 120/122 (98%) | 111 (92%) | 8 (7%)   | 1 (1%)   | 19          | 51  |
| 40  | Ai    | 95/97 (98%)   | 86 (90%)  | 9 (10%)  | 0        | 100         | 100 |
| 41  | Aj    | 82/84 (98%)   | 75 (92%)  | 7 (8%)   | 0        | 100         | 100 |
| 42  | Ak    | 67/69 (97%)   | 63 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 43  | Al    | 48/50 (96%)   | 44 (92%)  | 4 (8%)   | 0        | 100         | 100 |
| 44  | Am    | 48/50 (96%)   | 45 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 45  | An    | 23/25 (92%)   | 23 (100%) | 0        | 0        | 100         | 100 |
| 46  | Ao    | 103/105 (98%) | 93 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 47  | Ap    | 89/91 (98%)   | 80 (90%)  | 9 (10%)  | 0        | 100         | 100 |
| 48  | Aq    | 136/138 (99%) | 94 (69%)  | 38 (28%) | 4 (3%)   | 4           | 24  |
| 49  | At    | 120/122 (98%) | 102 (85%) | 16 (13%) | 2 (2%)   | 9           | 34  |
| 50  | Au    | 215/217 (99%) | 193 (90%) | 18 (8%)  | 4 (2%)   | 8           | 31  |
| 53  | BD    | 218/220 (99%) | 202 (93%) | 15 (7%)  | 1 (0%)   | 29          | 61  |
| 54  | BE    | 255/257 (99%) | 235 (92%) | 19 (8%)  | 1 (0%)   | 34          | 67  |
| 55  | BF    | 188/190 (99%) | 171 (91%) | 17 (9%)  | 0        | 100         | 100 |
| 56  | BG    | 230/232 (99%) | 208 (90%) | 21 (9%)  | 1 (0%)   | 34          | 67  |
| 57  | BH    | 181/183 (99%) | 166 (92%) | 14 (8%)  | 1 (1%)   | 25          | 57  |
| 58  | BI    | 205/207 (99%) | 175 (85%) | 26 (13%) | 4 (2%)   | 7           | 30  |
| 59  | BJ    | 177/179 (99%) | 151 (85%) | 25 (14%) | 1 (1%)   | 25          | 57  |
| 60  | BK    | 96/98 (98%)   | 82 (85%)  | 12 (12%) | 2 (2%)   | 7           | 30  |
| 61  | BL    | 151/153 (99%) | 132 (87%) | 18 (12%) | 1 (1%)   | 22          | 55  |
| 62  | BM    | 118/120 (98%) | 112 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 63  | BN    | 147/149 (99%) | 129 (88%) | 17 (12%) | 1 (1%)   | 22          | 55  |
| 64  | BO    | 134/136 (98%) | 119 (89%) | 13 (10%) | 2 (2%)   | 10          | 36  |
| 65  | BP    | 118/120 (98%) | 101 (86%) | 12 (10%) | 5 (4%)   | 3           | 18  |
| 66  | BQ    | 137/139 (99%) | 127 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 67  | BR    | 123/125 (98%) | 105 (85%) | 16 (13%) | 2 (2%)   | 9           | 34  |
| 68  | BS    | 137/139 (99%) | 118 (86%) | 16 (12%) | 3 (2%)   | 6           | 29  |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 69  | BT    | 141/143 (99%)     | 129 (92%)   | 11 (8%)   | 1 (1%)   | 22          | 55  |
| 70  | BU    | 95/97 (98%)       | 91 (96%)    | 4 (4%)    | 0        | 100         | 100 |
| 71  | BV    | 79/81 (98%)       | 75 (95%)    | 4 (5%)    | 0        | 100         | 100 |
| 72  | BW    | 127/129 (98%)     | 121 (95%)   | 6 (5%)    | 0        | 100         | 100 |
| 73  | BX    | 137/139 (99%)     | 124 (90%)   | 11 (8%)   | 2 (2%)   | 10          | 36  |
| 74  | BY    | 123/125 (98%)     | 108 (88%)   | 15 (12%)  | 0        | 100         | 100 |
| 75  | BZ    | 84/86 (98%)       | 74 (88%)    | 10 (12%)  | 0        | 100         | 100 |
| 76  | Ba    | 95/97 (98%)       | 87 (92%)    | 8 (8%)    | 0        | 100         | 100 |
| 77  | Bb    | 78/80 (98%)       | 71 (91%)    | 7 (9%)    | 0        | 100         | 100 |
| 78  | Bc    | 60/62 (97%)       | 55 (92%)    | 5 (8%)    | 0        | 100         | 100 |
| 79  | Bd    | 49/51 (96%)       | 43 (88%)    | 6 (12%)   | 0        | 100         | 100 |
| 80  | Be    | 53/55 (96%)       | 51 (96%)    | 2 (4%)    | 0        | 100         | 100 |
| 81  | Bf    | 71/73 (97%)       | 64 (90%)    | 6 (8%)    | 1 (1%)   | 11          | 37  |
| 82  | Bg    | 312/314 (99%)     | 281 (90%)   | 31 (10%)  | 0        | 100         | 100 |
| 85  | A     | 37/39 (95%)       | 20 (54%)    | 14 (38%)  | 3 (8%)   | 1           | 5   |
| All | All   | 11617/11838 (98%) | 10430 (90%) | 1084 (9%) | 103 (1%) | 21          | 49  |

All (103) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 196 | TRP  |
| 1   | AA    | 197 | PRO  |
| 1   | AA    | 201 | GLY  |
| 2   | BA    | 206 | ASP  |
| 5   | AC    | 148 | PRO  |
| 9   | AD    | 265 | ARG  |
| 10  | AE    | 133 | PHE  |
| 15  | AJ    | 57  | VAL  |
| 16  | AK    | 5   | ASP  |
| 16  | AK    | 25  | PRO  |
| 16  | AK    | 26  | LYS  |
| 16  | AK    | 72  | ASN  |
| 16  | AK    | 103 | LEU  |
| 16  | AK    | 104 | ALA  |
| 17  | AL    | 46  | ILE  |
| 17  | AL    | 47  | ALA  |
| 17  | AL    | 62  | PRO  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 17         | AL           | 172        | GLU         |
| 19         | AN           | 95         | ALA         |
| 23         | AR           | 112        | SER         |
| 26         | AU           | 61         | VAL         |
| 34         | Ac           | 102        | SER         |
| 37         | Af           | 106        | TYR         |
| 48         | Aq           | 22         | VAL         |
| 48         | Aq           | 58         | ILE         |
| 49         | At           | 17         | LEU         |
| 50         | Au           | 60         | ARG         |
| 50         | Au           | 164        | CYS         |
| 53         | BD           | 218        | LEU         |
| 58         | BI           | 133        | GLU         |
| 58         | BI           | 160        | SER         |
| 58         | BI           | 161        | LEU         |
| 68         | BS           | 89         | ASP         |
| 68         | BS           | 91         | LYS         |
| 2          | BA           | 203        | PHE         |
| 2          | BA           | 204        | TYR         |
| 5          | AC           | 53         | ALA         |
| 9          | AD           | 253        | TYR         |
| 17         | AL           | 136        | LYS         |
| 17         | AL           | 165        | LYS         |
| 50         | Au           | 24         | LYS         |
| 60         | BK           | 41         | PRO         |
| 64         | BO           | 21         | VAL         |
| 65         | BP           | 66         | GLU         |
| 68         | BS           | 87         | GLN         |
| 69         | BT           | 31         | PRO         |
| 85         | A            | 33         | ILE         |
| 9          | AD           | 258        | LYS         |
| 10         | AE           | 127        | SER         |
| 10         | AE           | 128        | HIS         |
| 13         | AH           | 117        | PHE         |
| 15         | AJ           | 56         | THR         |
| 17         | AL           | 64         | VAL         |
| 22         | AQ           | 161        | SER         |
| 26         | AU           | 60         | VAL         |
| 33         | Ab           | 25         | ARG         |
| 49         | At           | 16         | PHE         |
| 61         | BL           | 14         | PRO         |
| 63         | BN           | 23         | PRO         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 64         | BO           | 19         | PRO         |
| 65         | BP           | 52         | LYS         |
| 65         | BP           | 68         | PRO         |
| 65         | BP           | 125        | PRO         |
| 67         | BR           | 5          | ARG         |
| 2          | BA           | 209        | GLU         |
| 4          | BB           | 39         | PHE         |
| 4          | BB           | 52         | THR         |
| 16         | AK           | 3          | ARG         |
| 16         | AK           | 78         | LEU         |
| 17         | AL           | 5          | ARG         |
| 17         | AL           | 78         | LEU         |
| 25         | AT           | 18         | PRO         |
| 37         | Af           | 107        | PRO         |
| 57         | BH           | 115        | LYS         |
| 58         | BI           | 131        | PRO         |
| 59         | BJ           | 123        | ILE         |
| 60         | BK           | 28         | HIS         |
| 67         | BR           | 4          | VAL         |
| 73         | BX           | 136        | GLY         |
| 9          | AD           | 260        | GLU         |
| 13         | AH           | 3          | THR         |
| 16         | AK           | 82         | ILE         |
| 16         | AK           | 96         | THR         |
| 25         | AT           | 53         | PRO         |
| 34         | Ac           | 108        | MET         |
| 39         | Ah           | 87         | LYS         |
| 50         | Au           | 22         | GLN         |
| 54         | BE           | 150        | PRO         |
| 56         | BG           | 103        | ASP         |
| 65         | BP           | 126        | VAL         |
| 81         | Bf           | 88         | PRO         |
| 85         | A            | 36         | LEU         |
| 11         | AF           | 223        | LYS         |
| 28         | AW           | 59         | HIS         |
| 48         | Aq           | 88         | PRO         |
| 85         | A            | 29         | LEU         |
| 73         | BX           | 86         | PRO         |
| 10         | AE           | 185        | PRO         |
| 16         | AK           | 73         | PRO         |
| 37         | Af           | 60         | PRO         |
| 16         | AK           | 52         | VAL         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | AK    | 53  | VAL  |
| 48  | Aq    | 60  | VAL  |

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

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | AA    | 194/199 (98%)  | 190 (98%)  | 4 (2%)   | 53          | 76  |
| 2   | BA    | 180/180 (100%) | 176 (98%)  | 4 (2%)   | 52          | 75  |
| 3   | AB    | 343/343 (100%) | 338 (98%)  | 5 (2%)   | 65          | 82  |
| 4   | BB    | 193/193 (100%) | 190 (98%)  | 3 (2%)   | 62          | 81  |
| 5   | AC    | 302/302 (100%) | 295 (98%)  | 7 (2%)   | 50          | 74  |
| 6   | BC    | 188/188 (100%) | 184 (98%)  | 4 (2%)   | 53          | 76  |
| 9   | AD    | 248/248 (100%) | 233 (94%)  | 15 (6%)  | 19          | 49  |
| 10  | AE    | 174/174 (100%) | 163 (94%)  | 11 (6%)  | 18          | 47  |
| 11  | AF    | 203/203 (100%) | 200 (98%)  | 3 (2%)   | 65          | 82  |
| 12  | AG    | 199/199 (100%) | 199 (100%) | 0        | 100         | 100 |
| 13  | AH    | 170/170 (100%) | 166 (98%)  | 4 (2%)   | 49          | 74  |
| 14  | AI    | 178/179 (99%)  | 176 (99%)  | 2 (1%)   | 73          | 86  |
| 15  | AJ    | 142/142 (100%) | 139 (98%)  | 3 (2%)   | 53          | 76  |
| 16  | AK    | 95/95 (100%)   | 89 (94%)   | 6 (6%)   | 18          | 47  |
| 17  | AL    | 171/171 (100%) | 163 (95%)  | 8 (5%)   | 26          | 57  |
| 18  | AM    | 118/118 (100%) | 116 (98%)  | 2 (2%)   | 60          | 80  |
| 19  | AN    | 171/171 (100%) | 169 (99%)  | 2 (1%)   | 71          | 85  |
| 20  | AO    | 168/168 (100%) | 165 (98%)  | 3 (2%)   | 59          | 79  |
| 21  | AP    | 134/134 (100%) | 134 (100%) | 0        | 100         | 100 |
| 22  | AQ    | 164/164 (100%) | 158 (96%)  | 6 (4%)   | 34          | 62  |
| 23  | AR    | 160/160 (100%) | 158 (99%)  | 2 (1%)   | 69          | 84  |
| 24  | AS    | 156/156 (100%) | 156 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 25  | AT    | 138/138 (100%) | 138 (100%) | 0        | 100         | 100 |
| 26  | AU    | 89/89 (100%)   | 86 (97%)   | 3 (3%)   | 37          | 65  |
| 27  | AV    | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 28  | AW    | 100/100 (100%) | 99 (99%)   | 1 (1%)   | 76          | 88  |
| 29  | AX    | 105/105 (100%) | 105 (100%) | 0        | 100         | 100 |
| 30  | AY    | 119/119 (100%) | 118 (99%)  | 1 (1%)   | 81          | 91  |
| 31  | AZ    | 117/117 (100%) | 116 (99%)  | 1 (1%)   | 78          | 90  |
| 32  | Aa    | 120/120 (100%) | 119 (99%)  | 1 (1%)   | 81          | 91  |
| 33  | Ab    | 58/101 (57%)   | 52 (90%)   | 6 (10%)  | 7           | 26  |
| 34  | Ac    | 88/88 (100%)   | 83 (94%)   | 5 (6%)   | 20          | 50  |
| 35  | Ad    | 97/97 (100%)   | 97 (100%)  | 0        | 100         | 100 |
| 36  | Ae    | 115/115 (100%) | 115 (100%) | 0        | 100         | 100 |
| 37  | Af    | 88/88 (100%)   | 87 (99%)   | 1 (1%)   | 73          | 86  |
| 38  | Ag    | 98/98 (100%)   | 98 (100%)  | 0        | 100         | 100 |
| 39  | Ah    | 109/109 (100%) | 105 (96%)  | 4 (4%)   | 34          | 62  |
| 40  | Ai    | 83/83 (100%)   | 83 (100%)  | 0        | 100         | 100 |
| 41  | Aj    | 71/71 (100%)   | 69 (97%)   | 2 (3%)   | 43          | 70  |
| 42  | Ak    | 64/64 (100%)   | 63 (98%)   | 1 (2%)   | 62          | 81  |
| 43  | Al    | 47/47 (100%)   | 44 (94%)   | 3 (6%)   | 17          | 47  |
| 44  | Am    | 46/46 (100%)   | 45 (98%)   | 1 (2%)   | 52          | 75  |
| 45  | An    | 24/24 (100%)   | 24 (100%)  | 0        | 100         | 100 |
| 46  | Ao    | 93/93 (100%)   | 91 (98%)   | 2 (2%)   | 52          | 75  |
| 47  | Ap    | 74/74 (100%)   | 73 (99%)   | 1 (1%)   | 67          | 83  |
| 48  | Aq    | 114/114 (100%) | 105 (92%)  | 9 (8%)   | 12          | 39  |
| 49  | At    | 106/106 (100%) | 103 (97%)  | 3 (3%)   | 43          | 70  |
| 50  | Au    | 196/196 (100%) | 184 (94%)  | 12 (6%)  | 18          | 48  |
| 53  | BD    | 183/183 (100%) | 179 (98%)  | 4 (2%)   | 52          | 75  |
| 54  | BE    | 220/220 (100%) | 217 (99%)  | 3 (1%)   | 67          | 83  |
| 55  | BF    | 160/160 (100%) | 158 (99%)  | 2 (1%)   | 69          | 84  |
| 56  | BG    | 202/202 (100%) | 201 (100%) | 1 (0%)   | 88          | 94  |
| 57  | BH    | 164/164 (100%) | 164 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed           | Rotameric  | Outliers | Percentiles |     |
|-----|-------|--------------------|------------|----------|-------------|-----|
| 58  | BI    | 179/179 (100%)     | 175 (98%)  | 4 (2%)   | 52          | 75  |
| 59  | BJ    | 160/160 (100%)     | 157 (98%)  | 3 (2%)   | 57          | 78  |
| 60  | BK    | 89/89 (100%)       | 88 (99%)   | 1 (1%)   | 73          | 86  |
| 61  | BL    | 138/138 (100%)     | 137 (99%)  | 1 (1%)   | 84          | 92  |
| 62  | BM    | 102/102 (100%)     | 102 (100%) | 0        | 100         | 100 |
| 63  | BN    | 130/130 (100%)     | 129 (99%)  | 1 (1%)   | 81          | 91  |
| 64  | BO    | 106/106 (100%)     | 105 (99%)  | 1 (1%)   | 78          | 90  |
| 65  | BP    | 109/109 (100%)     | 100 (92%)  | 9 (8%)   | 11          | 36  |
| 66  | BQ    | 115/115 (100%)     | 114 (99%)  | 1 (1%)   | 78          | 90  |
| 67  | BR    | 113/113 (100%)     | 113 (100%) | 0        | 100         | 100 |
| 68  | BS    | 121/121 (100%)     | 114 (94%)  | 7 (6%)   | 20          | 50  |
| 69  | BT    | 113/113 (100%)     | 112 (99%)  | 1 (1%)   | 78          | 90  |
| 70  | BU    | 90/90 (100%)       | 90 (100%)  | 0        | 100         | 100 |
| 71  | BV    | 65/65 (100%)       | 63 (97%)   | 2 (3%)   | 40          | 68  |
| 72  | BW    | 112/112 (100%)     | 107 (96%)  | 5 (4%)   | 27          | 58  |
| 73  | BX    | 111/111 (100%)     | 108 (97%)  | 3 (3%)   | 44          | 70  |
| 74  | BY    | 107/107 (100%)     | 106 (99%)  | 1 (1%)   | 78          | 90  |
| 75  | BZ    | 75/75 (100%)       | 73 (97%)   | 2 (3%)   | 44          | 70  |
| 76  | Ba    | 84/84 (100%)       | 84 (100%)  | 0        | 100         | 100 |
| 77  | Bb    | 72/72 (100%)       | 71 (99%)   | 1 (1%)   | 67          | 83  |
| 78  | Bc    | 55/55 (100%)       | 53 (96%)   | 2 (4%)   | 35          | 63  |
| 79  | Bd    | 45/45 (100%)       | 45 (100%)  | 0        | 100         | 100 |
| 80  | Be    | 44/44 (100%)       | 41 (93%)   | 3 (7%)   | 16          | 45  |
| 81  | Bf    | 66/66 (100%)       | 66 (100%)  | 0        | 100         | 100 |
| 82  | Bg    | 272/272 (100%)     | 270 (99%)  | 2 (1%)   | 84          | 92  |
| All | All   | 10112/10161 (100%) | 9901 (98%) | 211 (2%) | 56          | 76  |

All (211) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 68  | ARG  |
| 1   | AA    | 193 | ARG  |
| 1   | AA    | 198 | ARG  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | AA           | 200        | ARG         |
| 2          | BA           | 42         | LYS         |
| 2          | BA           | 149        | ASN         |
| 2          | BA           | 205        | ARG         |
| 2          | BA           | 208        | GLU         |
| 3          | AB           | 17         | LEU         |
| 3          | AB           | 24         | ARG         |
| 3          | AB           | 66         | LYS         |
| 3          | AB           | 67         | VAL         |
| 3          | AB           | 294        | LYS         |
| 4          | BB           | 49         | VAL         |
| 4          | BB           | 52         | THR         |
| 4          | BB           | 76         | ASN         |
| 5          | AC           | 38         | ASN         |
| 5          | AC           | 48         | ASN         |
| 5          | AC           | 52         | TYR         |
| 5          | AC           | 95         | MET         |
| 5          | AC           | 152        | LEU         |
| 5          | AC           | 154        | VAL         |
| 5          | AC           | 215        | ASN         |
| 6          | BC           | 134        | ASN         |
| 6          | BC           | 255        | LEU         |
| 6          | BC           | 257        | LYS         |
| 6          | BC           | 259        | THR         |
| 9          | AD           | 6          | VAL         |
| 9          | AD           | 8          | LYS         |
| 9          | AD           | 9          | ASN         |
| 9          | AD           | 20         | PHE         |
| 9          | AD           | 21         | ARG         |
| 9          | AD           | 191        | ASN         |
| 9          | AD           | 235        | MET         |
| 9          | AD           | 255        | LYS         |
| 9          | AD           | 259        | LYS         |
| 9          | AD           | 260        | GLU         |
| 9          | AD           | 261        | VAL         |
| 9          | AD           | 262        | LYS         |
| 9          | AD           | 263        | LYS         |
| 9          | AD           | 264        | LYS         |
| 9          | AD           | 265        | ARG         |
| 10         | AE           | 128        | HIS         |
| 10         | AE           | 130        | LYS         |
| 10         | AE           | 131        | LYS         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 10         | AE           | 134        | SER         |
| 10         | AE           | 137        | VAL         |
| 10         | AE           | 138        | ARG         |
| 10         | AE           | 206        | VAL         |
| 10         | AE           | 207        | LYS         |
| 10         | AE           | 208        | ILE         |
| 10         | AE           | 223        | ARG         |
| 10         | AE           | 279        | ASN         |
| 11         | AF           | 146        | ASN         |
| 11         | AF           | 161        | LYS         |
| 11         | AF           | 166        | ARG         |
| 13         | AH           | 3          | THR         |
| 13         | AH           | 4          | ILE         |
| 13         | AH           | 5          | LEU         |
| 13         | AH           | 111        | LEU         |
| 14         | AI           | 69         | ARG         |
| 14         | AI           | 73         | ASN         |
| 15         | AJ           | 54         | ARG         |
| 15         | AJ           | 55         | TYR         |
| 15         | AJ           | 56         | THR         |
| 16         | AK           | 3          | ARG         |
| 16         | AK           | 4          | GLU         |
| 16         | AK           | 69         | LEU         |
| 16         | AK           | 71         | ASN         |
| 16         | AK           | 85         | ASN         |
| 16         | AK           | 101        | MET         |
| 17         | AL           | 46         | ILE         |
| 17         | AL           | 49         | ARG         |
| 17         | AL           | 63         | THR         |
| 17         | AL           | 130        | LYS         |
| 17         | AL           | 159        | ASN         |
| 17         | AL           | 165        | LYS         |
| 17         | AL           | 172        | GLU         |
| 17         | AL           | 175        | ASN         |
| 18         | AM           | 5          | ARG         |
| 18         | AM           | 46         | ARG         |
| 19         | AN           | 38         | ARG         |
| 19         | AN           | 183        | THR         |
| 20         | AO           | 65         | ASN         |
| 20         | AO           | 118        | MET         |
| 20         | AO           | 184        | ASN         |
| 22         | AQ           | 10         | ASP         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 22         | AQ           | 11         | ARG         |
| 22         | AQ           | 12         | LYS         |
| 22         | AQ           | 13         | VAL         |
| 22         | AQ           | 15         | ARG         |
| 22         | AQ           | 146        | ARG         |
| 23         | AR           | 113        | LYS         |
| 23         | AR           | 114        | LYS         |
| 26         | AU           | 50         | ASN         |
| 26         | AU           | 56         | LEU         |
| 26         | AU           | 97         | ARG         |
| 28         | AW           | 45         | ASN         |
| 30         | AY           | 36         | LYS         |
| 31         | AZ           | 59         | LYS         |
| 32         | Aa           | 87         | ARG         |
| 33         | Ab           | 22         | LYS         |
| 33         | Ab           | 23         | LYS         |
| 33         | Ab           | 26         | SER         |
| 33         | Ab           | 27         | GLN         |
| 33         | Ab           | 28         | ARG         |
| 33         | Ab           | 61         | ASN         |
| 34         | Ac           | 36         | LYS         |
| 34         | Ac           | 102        | SER         |
| 34         | Ac           | 105        | ILE         |
| 34         | Ac           | 106        | ARG         |
| 34         | Ac           | 107        | SER         |
| 37         | Af           | 108        | SER         |
| 39         | Ah           | 48         | ARG         |
| 39         | Ah           | 87         | LYS         |
| 39         | Ah           | 91         | MET         |
| 39         | Ah           | 92         | ARG         |
| 41         | Aj           | 65         | ARG         |
| 41         | Aj           | 67         | LEU         |
| 42         | Ak           | 21         | LYS         |
| 43         | Al           | 20         | ASN         |
| 43         | Al           | 21         | ARG         |
| 43         | Al           | 28         | ARG         |
| 44         | Am           | 120        | ASN         |
| 46         | Ao           | 3          | ASN         |
| 46         | Ao           | 98         | LYS         |
| 47         | Ap           | 84         | ARG         |
| 48         | Aq           | 8          | ASN         |
| 48         | Aq           | 22         | VAL         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 48         | Aq           | 31         | LYS         |
| 48         | Aq           | 35         | LEU         |
| 48         | Aq           | 58         | ILE         |
| 48         | Aq           | 59         | THR         |
| 48         | Aq           | 97         | ASN         |
| 48         | Aq           | 111        | ASN         |
| 48         | Aq           | 143        | VAL         |
| 49         | At           | 18         | ILE         |
| 49         | At           | 41         | ASN         |
| 49         | At           | 83         | ASN         |
| 50         | Au           | 21         | ASN         |
| 50         | Au           | 23         | ARG         |
| 50         | Au           | 54         | ARG         |
| 50         | Au           | 58         | THR         |
| 50         | Au           | 60         | ARG         |
| 50         | Au           | 143        | ASN         |
| 50         | Au           | 159        | MET         |
| 50         | Au           | 161        | LYS         |
| 50         | Au           | 162        | VAL         |
| 50         | Au           | 188        | ASN         |
| 50         | Au           | 197        | ASN         |
| 50         | Au           | 215        | ARG         |
| 53         | BD           | 64         | ARG         |
| 53         | BD           | 216        | GLU         |
| 53         | BD           | 217        | ILE         |
| 53         | BD           | 218        | LEU         |
| 54         | BE           | 75         | LYS         |
| 54         | BE           | 197        | ASN         |
| 54         | BE           | 230        | ASN         |
| 55         | BF           | 119        | SER         |
| 55         | BF           | 135        | ARG         |
| 56         | BG           | 202        | ASN         |
| 58         | BI           | 59         | ARG         |
| 58         | BI           | 132        | GLU         |
| 58         | BI           | 158        | ILE         |
| 58         | BI           | 159        | SER         |
| 59         | BJ           | 30         | LYS         |
| 59         | BJ           | 137        | VAL         |
| 59         | BJ           | 138        | ARG         |
| 60         | BK           | 96         | ARG         |
| 61         | BL           | 101        | ARG         |
| 63         | BN           | 104        | ARG         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 64         | BO           | 128        | ARG         |
| 65         | BP           | 45         | LEU         |
| 65         | BP           | 47         | ARG         |
| 65         | BP           | 49         | LEU         |
| 65         | BP           | 50         | ARG         |
| 65         | BP           | 51         | ARG         |
| 65         | BP           | 52         | LYS         |
| 65         | BP           | 66         | GLU         |
| 65         | BP           | 70         | MET         |
| 65         | BP           | 71         | GLU         |
| 66         | BQ           | 13         | PHE         |
| 68         | BS           | 17         | ASN         |
| 68         | BS           | 23         | ARG         |
| 68         | BS           | 66         | ARG         |
| 68         | BS           | 73         | ASN         |
| 68         | BS           | 87         | GLN         |
| 68         | BS           | 88         | LYS         |
| 68         | BS           | 91         | LYS         |
| 69         | BT           | 62         | ARG         |
| 71         | BV           | 41         | LYS         |
| 71         | BV           | 81         | LYS         |
| 72         | BW           | 5          | ASN         |
| 72         | BW           | 15         | ASN         |
| 72         | BW           | 96         | SER         |
| 72         | BW           | 97         | ARG         |
| 72         | BW           | 102        | ILE         |
| 73         | BX           | 127        | ASN         |
| 73         | BX           | 138        | LYS         |
| 73         | BX           | 139        | GLU         |
| 74         | BY           | 15         | ASN         |
| 75         | BZ           | 62         | VAL         |
| 75         | BZ           | 112        | ASN         |
| 77         | Bb           | 77         | CYS         |
| 78         | Bc           | 32         | VAL         |
| 78         | Bc           | 66         | ARG         |
| 80         | Be           | 18         | LYS         |
| 80         | Be           | 35         | ARG         |
| 80         | Be           | 52         | LYS         |
| 82         | Bg           | 96         | THR         |
| 82         | Bg           | 133        | ASN         |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 97  | ASN  |
| 1   | AA    | 132 | ASN  |
| 1   | AA    | 209 | HIS  |
| 1   | AA    | 218 | HIS  |
| 2   | BA    | 149 | ASN  |
| 3   | AB    | 68  | ASN  |
| 3   | AB    | 204 | GLN  |
| 3   | AB    | 322 | HIS  |
| 3   | AB    | 380 | GLN  |
| 4   | BB    | 40  | ASN  |
| 4   | BB    | 76  | ASN  |
| 5   | AC    | 215 | ASN  |
| 5   | AC    | 343 | GLN  |
| 6   | BC    | 134 | ASN  |
| 9   | AD    | 17  | GLN  |
| 9   | AD    | 191 | ASN  |
| 9   | AD    | 198 | HIS  |
| 10  | AE    | 190 | HIS  |
| 10  | AE    | 266 | GLN  |
| 10  | AE    | 279 | ASN  |
| 11  | AF    | 116 | GLN  |
| 11  | AF    | 146 | ASN  |
| 11  | AF    | 226 | HIS  |
| 12  | AG    | 43  | GLN  |
| 14  | AI    | 14  | ASN  |
| 14  | AI    | 51  | HIS  |
| 14  | AI    | 147 | HIS  |
| 15  | AJ    | 167 | GLN  |
| 16  | AK    | 12  | ASN  |
| 16  | AK    | 68  | HIS  |
| 17  | AL    | 19  | GLN  |
| 17  | AL    | 67  | HIS  |
| 17  | AL    | 159 | ASN  |
| 17  | AL    | 175 | ASN  |
| 18  | AM    | 56  | GLN  |
| 18  | AM    | 78  | GLN  |
| 19  | AN    | 87  | HIS  |
| 19  | AN    | 201 | HIS  |
| 20  | AO    | 14  | HIS  |
| 20  | AO    | 50  | ASN  |
| 20  | AO    | 65  | ASN  |
| 20  | AO    | 96  | GLN  |
| 20  | AO    | 184 | ASN  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 21         | AP           | 40         | HIS         |
| 21         | AP           | 80         | GLN         |
| 21         | AP           | 97         | ASN         |
| 24         | AS           | 66         | GLN         |
| 24         | AS           | 91         | HIS         |
| 25         | AT           | 22         | HIS         |
| 26         | AU           | 50         | ASN         |
| 26         | AU           | 55         | ASN         |
| 27         | AV           | 101        | ASN         |
| 28         | AW           | 45         | ASN         |
| 30         | AY           | 56         | GLN         |
| 30         | AY           | 61         | HIS         |
| 30         | AY           | 86         | GLN         |
| 32         | Aa           | 60         | HIS         |
| 33         | Ab           | 12         | GLN         |
| 33         | Ab           | 27         | GLN         |
| 33         | Ab           | 61         | ASN         |
| 35         | Ad           | 28         | ASN         |
| 37         | Af           | 99         | HIS         |
| 38         | Ag           | 73         | HIS         |
| 39         | Ah           | 63         | GLN         |
| 40         | Ai           | 36         | HIS         |
| 41         | Aj           | 57         | ASN         |
| 43         | Al           | 20         | ASN         |
| 44         | Am           | 90         | ASN         |
| 44         | Am           | 120        | ASN         |
| 46         | Ao           | 3          | ASN         |
| 46         | Ao           | 19         | GLN         |
| 46         | Ao           | 36         | GLN         |
| 48         | Aq           | 8          | ASN         |
| 48         | Aq           | 97         | ASN         |
| 48         | Aq           | 103        | ASN         |
| 48         | Aq           | 111        | ASN         |
| 49         | At           | 36         | ASN         |
| 49         | At           | 100        | ASN         |
| 50         | Au           | 22         | GLN         |
| 50         | Au           | 84         | HIS         |
| 50         | Au           | 143        | ASN         |
| 50         | Au           | 197        | ASN         |
| 53         | BD           | 101        | GLN         |
| 54         | BE           | 8          | HIS         |
| 54         | BE           | 98         | HIS         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 54         | BE           | 161        | GLN         |
| 54         | BE           | 197        | ASN         |
| 54         | BE           | 230        | ASN         |
| 55         | BF           | 65         | GLN         |
| 55         | BF           | 82         | ASN         |
| 55         | BF           | 114        | ASN         |
| 56         | BG           | 81         | HIS         |
| 56         | BG           | 202        | ASN         |
| 56         | BG           | 227        | GLN         |
| 61         | BL           | 83         | GLN         |
| 62         | BM           | 73         | GLN         |
| 63         | BN           | 105        | ASN         |
| 65         | BP           | 41         | GLN         |
| 65         | BP           | 103        | ASN         |
| 65         | BP           | 128        | HIS         |
| 66         | BQ           | 24         | HIS         |
| 66         | BQ           | 80         | GLN         |
| 66         | BQ           | 86         | GLN         |
| 67         | BR           | 62         | GLN         |
| 68         | BS           | 17         | ASN         |
| 68         | BS           | 42         | HIS         |
| 69         | BT           | 91         | HIS         |
| 72         | BW           | 5          | ASN         |
| 72         | BW           | 15         | ASN         |
| 72         | BW           | 16         | ASN         |
| 72         | BW           | 44         | HIS         |
| 72         | BW           | 56         | HIS         |
| 72         | BW           | 70         | ASN         |
| 72         | BW           | 90         | GLN         |
| 72         | BW           | 98         | GLN         |
| 73         | BX           | 127        | ASN         |
| 74         | BY           | 15         | ASN         |
| 74         | BY           | 29         | HIS         |
| 74         | BY           | 89         | HIS         |
| 75         | BZ           | 106        | GLN         |
| 75         | BZ           | 112        | ASN         |
| 78         | Bc           | 24         | GLN         |
| 78         | Bc           | 26         | GLN         |
| 78         | Bc           | 29         | GLN         |
| 80         | Be           | 39         | ASN         |
| 82         | Bg           | 133        | ASN         |
| 82         | Bg           | 159        | ASN         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 82  | Bg    | 296 | GLN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 51  | A2    | 3600/3612 (99%) | 863 (23%)         | 15 (0%)         |
| 52  | B1    | 1701/1708 (99%) | 408 (23%)         | 10 (0%)         |
| 7   | A3    | 156/157 (99%)   | 40 (25%)          | 3 (1%)          |
| 8   | A4    | 118/119 (99%)   | 22 (18%)          | 0               |
| 83  | Bv    | 75/76 (98%)     | 23 (30%)          | 0               |
| 84  | Bx    | 15/16 (93%)     | 10 (66%)          | 0               |
| All | All   | 5665/5688 (99%) | 1366 (24%)        | 28 (0%)         |

All (1366) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A3    | 16  | G    |
| 7   | A3    | 23  | C    |
| 7   | A3    | 33  | G    |
| 7   | A3    | 34  | U    |
| 7   | A3    | 35  | C    |
| 7   | A3    | 39  | G    |
| 7   | A3    | 52  | A    |
| 7   | A3    | 59  | A    |
| 7   | A3    | 63  | U    |
| 7   | A3    | 72  | A    |
| 7   | A3    | 80  | A    |
| 7   | A3    | 81  | C    |
| 7   | A3    | 82  | A    |
| 7   | A3    | 83  | C    |
| 7   | A3    | 84  | A    |
| 7   | A3    | 87  | G    |
| 7   | A3    | 88  | A    |
| 7   | A3    | 94  | G    |
| 7   | A3    | 95  | A    |
| 7   | A3    | 103 | A    |
| 7   | A3    | 105 | C    |
| 7   | A3    | 107 | C    |
| 7   | A3    | 108 | A    |
| 7   | A3    | 109 | C    |
| 7   | A3    | 110 | U    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 7          | A3           | 111        | U           |
| 7          | A3           | 112        | G           |
| 7          | A3           | 114        | G           |
| 7          | A3           | 120        | G           |
| 7          | A3           | 121        | G           |
| 7          | A3           | 123        | U           |
| 7          | A3           | 124        | U           |
| 7          | A3           | 125        | C           |
| 7          | A3           | 127        | U           |
| 7          | A3           | 128        | C           |
| 7          | A3           | 129        | C           |
| 7          | A3           | 130        | C           |
| 7          | A3           | 148        | A           |
| 7          | A3           | 151        | G           |
| 7          | A3           | 157        | U           |
| 8          | A4           | 7          | G           |
| 8          | A4           | 10         | C           |
| 8          | A4           | 11         | A           |
| 8          | A4           | 14         | C           |
| 8          | A4           | 22         | A           |
| 8          | A4           | 27         | G           |
| 8          | A4           | 29         | C           |
| 8          | A4           | 33         | U           |
| 8          | A4           | 47         | G           |
| 8          | A4           | 48         | G           |
| 8          | A4           | 53         | U           |
| 8          | A4           | 54         | A           |
| 8          | A4           | 59         | G           |
| 8          | A4           | 63         | C           |
| 8          | A4           | 64         | G           |
| 8          | A4           | 76         | U           |
| 8          | A4           | 89         | G           |
| 8          | A4           | 91         | C           |
| 8          | A4           | 97         | G           |
| 8          | A4           | 108        | G           |
| 8          | A4           | 110        | G           |
| 8          | A4           | 119        | U           |
| 51         | A2           | 6          | C           |
| 51         | A2           | 9          | C           |
| 51         | A2           | 10         | A           |
| 51         | A2           | 14         | C           |
| 51         | A2           | 22         | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 23         | C           |
| 51         | A2           | 25         | A           |
| 51         | A2           | 32         | G           |
| 51         | A2           | 39         | A           |
| 51         | A2           | 42         | A           |
| 51         | A2           | 47         | A           |
| 51         | A2           | 48         | G           |
| 51         | A2           | 49         | U           |
| 51         | A2           | 55         | G           |
| 51         | A2           | 59         | A           |
| 51         | A2           | 64         | A           |
| 51         | A2           | 65         | A           |
| 51         | A2           | 71         | C           |
| 51         | A2           | 72         | C           |
| 51         | A2           | 73         | A           |
| 51         | A2           | 76         | A           |
| 51         | A2           | 84         | A           |
| 51         | A2           | 91         | G           |
| 51         | A2           | 101        | A           |
| 51         | A2           | 110        | C           |
| 51         | A2           | 116        | G           |
| 51         | A2           | 119        | G           |
| 51         | A2           | 120        | A           |
| 51         | A2           | 121        | A           |
| 51         | A2           | 131        | C           |
| 51         | A2           | 132        | G           |
| 51         | A2           | 133        | C           |
| 51         | A2           | 134        | G           |
| 51         | A2           | 140        | C           |
| 51         | A2           | 141        | G           |
| 51         | A2           | 143        | G           |
| 51         | A2           | 147        | U           |
| 51         | A2           | 149        | U           |
| 51         | A2           | 150        | G           |
| 51         | A2           | 155        | A           |
| 51         | A2           | 156        | C           |
| 51         | A2           | 157        | G           |
| 51         | A2           | 167        | C           |
| 51         | A2           | 169        | C           |
| 51         | A2           | 179        | G           |
| 51         | A2           | 180        | C           |
| 51         | A2           | 181        | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 182        | C           |
| 51         | A2           | 183        | G           |
| 51         | A2           | 184        | U           |
| 51         | A2           | 185        | G           |
| 51         | A2           | 186        | G           |
| 51         | A2           | 189        | G           |
| 51         | A2           | 193        | C           |
| 51         | A2           | 196        | G           |
| 51         | A2           | 197        | U           |
| 51         | A2           | 199        | C           |
| 51         | A2           | 201        | U           |
| 51         | A2           | 206        | U           |
| 51         | A2           | 212        | C           |
| 51         | A2           | 213        | C           |
| 51         | A2           | 214        | C           |
| 51         | A2           | 215        | A           |
| 51         | A2           | 222        | G           |
| 51         | A2           | 227        | G           |
| 51         | A2           | 228        | U           |
| 51         | A2           | 229        | G           |
| 51         | A2           | 230        | U           |
| 51         | A2           | 231        | G           |
| 51         | A2           | 234        | G           |
| 51         | A2           | 237        | G           |
| 51         | A2           | 250        | G           |
| 51         | A2           | 251        | G           |
| 51         | A2           | 252        | C           |
| 51         | A2           | 253        | G           |
| 51         | A2           | 257        | G           |
| 51         | A2           | 258        | C           |
| 51         | A2           | 260        | C           |
| 51         | A2           | 261        | G           |
| 51         | A2           | 275        | U           |
| 51         | A2           | 286        | G           |
| 51         | A2           | 291        | U           |
| 51         | A2           | 300        | A           |
| 51         | A2           | 303        | C           |
| 51         | A2           | 309        | G           |
| 51         | A2           | 310        | U           |
| 51         | A2           | 311        | A           |
| 51         | A2           | 334        | C           |
| 51         | A2           | 338        | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 341        | A           |
| 51         | A2           | 348        | U           |
| 51         | A2           | 351        | U           |
| 51         | A2           | 354        | A           |
| 51         | A2           | 357        | A           |
| 51         | A2           | 367        | G           |
| 51         | A2           | 370        | A           |
| 51         | A2           | 375        | U           |
| 51         | A2           | 379        | A           |
| 51         | A2           | 381        | G           |
| 51         | A2           | 390        | A           |
| 51         | A2           | 402        | A           |
| 51         | A2           | 406        | G           |
| 51         | A2           | 407        | G           |
| 51         | A2           | 409        | G           |
| 51         | A2           | 425        | G           |
| 51         | A2           | 426        | U           |
| 51         | A2           | 434        | U           |
| 51         | A2           | 444        | G           |
| 51         | A2           | 446        | A           |
| 51         | A2           | 447        | G           |
| 51         | A2           | 448        | U           |
| 51         | A2           | 449        | C           |
| 51         | A2           | 457        | A           |
| 51         | A2           | 460        | A           |
| 51         | A2           | 469        | G           |
| 51         | A2           | 479        | C           |
| 51         | A2           | 480        | C           |
| 51         | A2           | 482        | G           |
| 51         | A2           | 483        | C           |
| 51         | A2           | 492        | C           |
| 51         | A2           | 494        | G           |
| 51         | A2           | 495        | C           |
| 51         | A2           | 496        | C           |
| 51         | A2           | 497        | C           |
| 51         | A2           | 498        | G           |
| 51         | A2           | 504        | U           |
| 51         | A2           | 505        | C           |
| 51         | A2           | 507        | U           |
| 51         | A2           | 508        | U           |
| 51         | A2           | 509        | C           |
| 51         | A2           | 513        | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 635        | G           |
| 51         | A2           | 641        | G           |
| 51         | A2           | 643        | A           |
| 51         | A2           | 645        | C           |
| 51         | A2           | 648        | C           |
| 51         | A2           | 649        | C           |
| 51         | A2           | 658        | G           |
| 51         | A2           | 661        | G           |
| 51         | A2           | 662        | A           |
| 51         | A2           | 674        | C           |
| 51         | A2           | 676        | G           |
| 51         | A2           | 677        | G           |
| 51         | A2           | 678        | C           |
| 51         | A2           | 680        | C           |
| 51         | A2           | 691        | G           |
| 51         | A2           | 692        | G           |
| 51         | A2           | 693        | U           |
| 51         | A2           | 695        | C           |
| 51         | A2           | 714        | A           |
| 51         | A2           | 720        | G           |
| 51         | A2           | 721        | G           |
| 51         | A2           | 724        | A           |
| 51         | A2           | 728        | C           |
| 51         | A2           | 731        | G           |
| 51         | A2           | 732        | C           |
| 51         | A2           | 737        | A           |
| 51         | A2           | 738        | A           |
| 51         | A2           | 739        | G           |
| 51         | A2           | 741        | U           |
| 51         | A2           | 902        | A           |
| 51         | A2           | 905        | G           |
| 51         | A2           | 906        | C           |
| 51         | A2           | 907        | C           |
| 51         | A2           | 913        | G           |
| 51         | A2           | 918        | C           |
| 51         | A2           | 919        | A           |
| 51         | A2           | 922        | A           |
| 51         | A2           | 923        | C           |
| 51         | A2           | 924        | U           |
| 51         | A2           | 925        | C           |
| 51         | A2           | 926        | G           |
| 51         | A2           | 927        | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 929        | G           |
| 51         | A2           | 931        | A           |
| 51         | A2           | 932        | U           |
| 51         | A2           | 933        | C           |
| 51         | A2           | 934        | C           |
| 51         | A2           | 944        | G           |
| 51         | A2           | 947        | A           |
| 51         | A2           | 948        | G           |
| 51         | A2           | 949        | C           |
| 51         | A2           | 950        | G           |
| 51         | A2           | 951        | A           |
| 51         | A2           | 952        | G           |
| 51         | A2           | 953        | A           |
| 51         | A2           | 954        | C           |
| 51         | A2           | 955        | C           |
| 51         | A2           | 956        | C           |
| 51         | A2           | 958        | U           |
| 51         | A2           | 960        | G           |
| 51         | A2           | 962        | C           |
| 51         | A2           | 967        | U           |
| 51         | A2           | 968        | C           |
| 51         | A2           | 969        | U           |
| 51         | A2           | 1053       | G           |
| 51         | A2           | 1055       | C           |
| 51         | A2           | 1062       | C           |
| 51         | A2           | 1066       | U           |
| 51         | A2           | 1067       | C           |
| 51         | A2           | 1078       | A           |
| 51         | A2           | 1083       | U           |
| 51         | A2           | 1084       | C           |
| 51         | A2           | 1086       | C           |
| 51         | A2           | 1087       | C           |
| 51         | A2           | 1147       | G           |
| 51         | A2           | 1149       | G           |
| 51         | A2           | 1150       | C           |
| 51         | A2           | 1152       | G           |
| 51         | A2           | 1156       | G           |
| 51         | A2           | 1161       | G           |
| 51         | A2           | 1162       | U           |
| 51         | A2           | 1163       | C           |
| 51         | A2           | 1164       | C           |
| 51         | A2           | 1165       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 1167       | A           |
| 51         | A2           | 1176       | C           |
| 51         | A2           | 1179       | G           |
| 51         | A2           | 1181       | G           |
| 51         | A2           | 1188       | G           |
| 51         | A2           | 1190       | C           |
| 51         | A2           | 1191       | G           |
| 51         | A2           | 1192       | U           |
| 51         | A2           | 1193       | C           |
| 51         | A2           | 1196       | G           |
| 51         | A2           | 1201       | G           |
| 51         | A2           | 1202       | G           |
| 51         | A2           | 1220       | C           |
| 51         | A2           | 1221       | A           |
| 51         | A2           | 1222       | C           |
| 51         | A2           | 1223       | G           |
| 51         | A2           | 1225       | G           |
| 51         | A2           | 1226       | C           |
| 51         | A2           | 1229       | G           |
| 51         | A2           | 1247       | C           |
| 51         | A2           | 1248       | G           |
| 51         | A2           | 1249       | G           |
| 51         | A2           | 1250       | C           |
| 51         | A2           | 1251       | G           |
| 51         | A2           | 1254       | G           |
| 51         | A2           | 1256       | G           |
| 51         | A2           | 1257       | A           |
| 51         | A2           | 1259       | C           |
| 51         | A2           | 1263       | C           |
| 51         | A2           | 1265       | G           |
| 51         | A2           | 1266       | G           |
| 51         | A2           | 1267       | G           |
| 51         | A2           | 1268       | U           |
| 51         | A2           | 1269       | C           |
| 51         | A2           | 1271       | G           |
| 51         | A2           | 1274       | G           |
| 51         | A2           | 1277       | A           |
| 51         | A2           | 1278       | C           |
| 51         | A2           | 1284       | C           |
| 51         | A2           | 1285       | U           |
| 51         | A2           | 1286       | A           |
| 51         | A2           | 1288       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 1296       | C           |
| 51         | A2           | 1303       | U           |
| 51         | A2           | 1309       | A           |
| 51         | A2           | 1337       | A           |
| 51         | A2           | 1341       | G           |
| 51         | A2           | 1342       | G           |
| 51         | A2           | 1343       | G           |
| 51         | A2           | 1348       | C           |
| 51         | A2           | 1349       | G           |
| 51         | A2           | 1350       | C           |
| 51         | A2           | 1353       | G           |
| 51         | A2           | 1360       | G           |
| 51         | A2           | 1361       | C           |
| 51         | A2           | 1362       | C           |
| 51         | A2           | 1364       | U           |
| 51         | A2           | 1370       | A           |
| 51         | A2           | 1373       | G           |
| 51         | A2           | 1374       | A           |
| 51         | A2           | 1377       | G           |
| 51         | A2           | 1380       | A           |
| 51         | A2           | 1381       | A           |
| 51         | A2           | 1392       | C           |
| 51         | A2           | 1393       | U           |
| 51         | A2           | 1394       | C           |
| 51         | A2           | 1403       | A           |
| 51         | A2           | 1421       | U           |
| 51         | A2           | 1423       | U           |
| 51         | A2           | 1426       | A           |
| 51         | A2           | 1429       | C           |
| 51         | A2           | 1430       | C           |
| 51         | A2           | 1433       | C           |
| 51         | A2           | 1463       | C           |
| 51         | A2           | 1464       | G           |
| 51         | A2           | 1465       | C           |
| 51         | A2           | 1466       | G           |
| 51         | A2           | 1467       | C           |
| 51         | A2           | 1468       | C           |
| 51         | A2           | 1472       | G           |
| 51         | A2           | 1479       | A           |
| 51         | A2           | 1480       | G           |
| 51         | A2           | 1483       | C           |
| 51         | A2           | 1485       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 1499       | G           |
| 51         | A2           | 1500       | A           |
| 51         | A2           | 1501       | C           |
| 51         | A2           | 1505       | A           |
| 51         | A2           | 1506       | A           |
| 51         | A2           | 1507       | A           |
| 51         | A2           | 1516       | A           |
| 51         | A2           | 1517       | C           |
| 51         | A2           | 1525       | G           |
| 51         | A2           | 1531       | G           |
| 51         | A2           | 1548       | C           |
| 51         | A2           | 1556       | G           |
| 51         | A2           | 1559       | G           |
| 51         | A2           | 1563       | G           |
| 51         | A2           | 1573       | U           |
| 51         | A2           | 1578       | U           |
| 51         | A2           | 1579       | G           |
| 51         | A2           | 1583       | A           |
| 51         | A2           | 1589       | C           |
| 51         | A2           | 1595       | A           |
| 51         | A2           | 1606       | G           |
| 51         | A2           | 1607       | G           |
| 51         | A2           | 1608       | G           |
| 51         | A2           | 1613       | A           |
| 51         | A2           | 1615       | G           |
| 51         | A2           | 1616       | A           |
| 51         | A2           | 1620       | A           |
| 51         | A2           | 1623       | G           |
| 51         | A2           | 1631       | U           |
| 51         | A2           | 1632       | A           |
| 51         | A2           | 1636       | G           |
| 51         | A2           | 1642       | U           |
| 51         | A2           | 1643       | C           |
| 51         | A2           | 1652       | G           |
| 51         | A2           | 1661       | A           |
| 51         | A2           | 1663       | G           |
| 51         | A2           | 1666       | A           |
| 51         | A2           | 1673       | G           |
| 51         | A2           | 1679       | G           |
| 51         | A2           | 1680       | C           |
| 51         | A2           | 1701       | A           |
| 51         | A2           | 1706       | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 1711       | A           |
| 51         | A2           | 1713       | C           |
| 51         | A2           | 1717       | U           |
| 51         | A2           | 1722       | C           |
| 51         | A2           | 1723       | G           |
| 51         | A2           | 1728       | A           |
| 51         | A2           | 1736       | U           |
| 51         | A2           | 1737       | C           |
| 51         | A2           | 1746       | G           |
| 51         | A2           | 1747       | A           |
| 51         | A2           | 1748       | A           |
| 51         | A2           | 1751       | G           |
| 51         | A2           | 1762       | A           |
| 51         | A2           | 1763       | U           |
| 51         | A2           | 1767       | C           |
| 51         | A2           | 1769       | A           |
| 51         | A2           | 1776       | A           |
| 51         | A2           | 1779       | G           |
| 51         | A2           | 1785       | G           |
| 51         | A2           | 1786       | A           |
| 51         | A2           | 1787       | A           |
| 51         | A2           | 1788       | G           |
| 51         | A2           | 1794       | C           |
| 51         | A2           | 1814       | G           |
| 51         | A2           | 1815       | U           |
| 51         | A2           | 1816       | G           |
| 51         | A2           | 1817       | G           |
| 51         | A2           | 1818       | A           |
| 51         | A2           | 1822       | C           |
| 51         | A2           | 1823       | G           |
| 51         | A2           | 1835       | G           |
| 51         | A2           | 1836       | G           |
| 51         | A2           | 1850       | G           |
| 51         | A2           | 1862       | C           |
| 51         | A2           | 1863       | U           |
| 51         | A2           | 1869       | A           |
| 51         | A2           | 1873       | A           |
| 51         | A2           | 1880       | G           |
| 51         | A2           | 1896       | C           |
| 51         | A2           | 1897       | G           |
| 51         | A2           | 1902       | C           |
| 51         | A2           | 1903       | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 1906       | G           |
| 51         | A2           | 1911       | U           |
| 51         | A2           | 1912       | C           |
| 51         | A2           | 1913       | A           |
| 51         | A2           | 1920       | A           |
| 51         | A2           | 1921       | G           |
| 51         | A2           | 1928       | U           |
| 51         | A2           | 1929       | G           |
| 51         | A2           | 1930       | U           |
| 51         | A2           | 1932       | G           |
| 51         | A2           | 1939       | A           |
| 51         | A2           | 1940       | U           |
| 51         | A2           | 1941       | A           |
| 51         | A2           | 1942       | G           |
| 51         | A2           | 1943       | A           |
| 51         | A2           | 1945       | A           |
| 51         | A2           | 1956       | G           |
| 51         | A2           | 1959       | C           |
| 51         | A2           | 1961       | U           |
| 51         | A2           | 1962       | G           |
| 51         | A2           | 1963       | G           |
| 51         | A2           | 1964       | A           |
| 51         | A2           | 1965       | A           |
| 51         | A2           | 1968       | C           |
| 51         | A2           | 1973       | U           |
| 51         | A2           | 1974       | C           |
| 51         | A2           | 1978       | U           |
| 51         | A2           | 1979       | A           |
| 51         | A2           | 1980       | A           |
| 51         | A2           | 1982       | G           |
| 51         | A2           | 1983       | A           |
| 51         | A2           | 1984       | G           |
| 51         | A2           | 1985       | U           |
| 51         | A2           | 1989       | U           |
| 51         | A2           | 1991       | A           |
| 51         | A2           | 2000       | C           |
| 51         | A2           | 2003       | C           |
| 51         | A2           | 2007       | A           |
| 51         | A2           | 2015       | G           |
| 51         | A2           | 2025       | U           |
| 51         | A2           | 2027       | G           |
| 51         | A2           | 2029       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 2033       | G           |
| 51         | A2           | 2035       | U           |
| 51         | A2           | 2036       | G           |
| 51         | A2           | 2037       | G           |
| 51         | A2           | 2043       | C           |
| 51         | A2           | 2050       | A           |
| 51         | A2           | 2246       | U           |
| 51         | A2           | 2247       | A           |
| 51         | A2           | 2251       | C           |
| 51         | A2           | 2268       | C           |
| 51         | A2           | 2279       | A           |
| 51         | A2           | 2280       | G           |
| 51         | A2           | 2282       | C           |
| 51         | A2           | 2283       | U           |
| 51         | A2           | 2284       | U           |
| 51         | A2           | 2285       | G           |
| 51         | A2           | 2292       | A           |
| 51         | A2           | 2301       | G           |
| 51         | A2           | 2310       | G           |
| 51         | A2           | 2324       | G           |
| 51         | A2           | 2325       | C           |
| 51         | A2           | 2327       | G           |
| 51         | A2           | 2330       | C           |
| 51         | A2           | 2339       | A           |
| 51         | A2           | 2340       | G           |
| 51         | A2           | 2358       | A           |
| 51         | A2           | 2363       | U           |
| 51         | A2           | 2374       | A           |
| 51         | A2           | 2377       | U           |
| 51         | A2           | 2389       | C           |
| 51         | A2           | 2397       | A           |
| 51         | A2           | 2400       | G           |
| 51         | A2           | 2401       | C           |
| 51         | A2           | 2416       | C           |
| 51         | A2           | 2420       | C           |
| 51         | A2           | 2426       | U           |
| 51         | A2           | 2429       | G           |
| 51         | A2           | 2442       | G           |
| 51         | A2           | 2450       | G           |
| 51         | A2           | 2451       | A           |
| 51         | A2           | 2453       | G           |
| 51         | A2           | 2467       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 2469       | U           |
| 51         | A2           | 2470       | C           |
| 51         | A2           | 2474       | U           |
| 51         | A2           | 2482       | G           |
| 51         | A2           | 2483       | C           |
| 51         | A2           | 2485       | G           |
| 51         | A2           | 2490       | A           |
| 51         | A2           | 2492       | A           |
| 51         | A2           | 2521       | G           |
| 51         | A2           | 2524       | U           |
| 51         | A2           | 2525       | G           |
| 51         | A2           | 2527       | C           |
| 51         | A2           | 2532       | A           |
| 51         | A2           | 2533       | U           |
| 51         | A2           | 2557       | G           |
| 51         | A2           | 2565       | G           |
| 51         | A2           | 2566       | A           |
| 51         | A2           | 2568       | C           |
| 51         | A2           | 2579       | A           |
| 51         | A2           | 2580       | A           |
| 51         | A2           | 2584       | G           |
| 51         | A2           | 2585       | G           |
| 51         | A2           | 2600       | A           |
| 51         | A2           | 2606       | C           |
| 51         | A2           | 2617       | G           |
| 51         | A2           | 2619       | G           |
| 51         | A2           | 2632       | C           |
| 51         | A2           | 2637       | G           |
| 51         | A2           | 2638       | A           |
| 51         | A2           | 2648       | C           |
| 51         | A2           | 2665       | G           |
| 51         | A2           | 2666       | U           |
| 51         | A2           | 2673       | G           |
| 51         | A2           | 2674       | A           |
| 51         | A2           | 2675       | A           |
| 51         | A2           | 2676       | A           |
| 51         | A2           | 2682       | G           |
| 51         | A2           | 2689       | C           |
| 51         | A2           | 2690       | G           |
| 51         | A2           | 2691       | G           |
| 51         | A2           | 2698       | C           |
| 51         | A2           | 2699       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 2700       | G           |
| 51         | A2           | 2704       | A           |
| 51         | A2           | 2705       | G           |
| 51         | A2           | 2706       | C           |
| 51         | A2           | 2717       | C           |
| 51         | A2           | 2718       | C           |
| 51         | A2           | 2719       | U           |
| 51         | A2           | 2720       | U           |
| 51         | A2           | 2722       | A           |
| 51         | A2           | 2723       | A           |
| 51         | A2           | 2732       | G           |
| 51         | A2           | 2739       | G           |
| 51         | A2           | 2740       | U           |
| 51         | A2           | 2741       | G           |
| 51         | A2           | 2746       | U           |
| 51         | A2           | 2748       | U           |
| 51         | A2           | 2751       | C           |
| 51         | A2           | 2766       | A           |
| 51         | A2           | 2767       | U           |
| 51         | A2           | 2769       | U           |
| 51         | A2           | 2773       | C           |
| 51         | A2           | 2776       | C           |
| 51         | A2           | 2778       | G           |
| 51         | A2           | 2781       | C           |
| 51         | A2           | 2785       | A           |
| 51         | A2           | 2793       | C           |
| 51         | A2           | 2798       | U           |
| 51         | A2           | 2801       | G           |
| 51         | A2           | 2804       | A           |
| 51         | A2           | 2805       | U           |
| 51         | A2           | 2806       | G           |
| 51         | A2           | 2817       | G           |
| 51         | A2           | 2819       | A           |
| 51         | A2           | 2825       | G           |
| 51         | A2           | 2839       | C           |
| 51         | A2           | 2860       | A           |
| 51         | A2           | 2871       | C           |
| 51         | A2           | 2876       | G           |
| 51         | A2           | 2881       | G           |
| 51         | A2           | 3586       | G           |
| 51         | A2           | 3587       | U           |
| 51         | A2           | 3588       | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 3589       | C           |
| 51         | A2           | 3591       | G           |
| 51         | A2           | 3596       | G           |
| 51         | A2           | 3597       | G           |
| 51         | A2           | 3601       | A           |
| 51         | A2           | 3606       | A           |
| 51         | A2           | 3614       | A           |
| 51         | A2           | 3615       | U           |
| 51         | A2           | 3616       | U           |
| 51         | A2           | 3620       | A           |
| 51         | A2           | 3627       | A           |
| 51         | A2           | 3633       | A           |
| 51         | A2           | 3643       | G           |
| 51         | A2           | 3644       | C           |
| 51         | A2           | 3651       | U           |
| 51         | A2           | 3672       | C           |
| 51         | A2           | 3676       | G           |
| 51         | A2           | 3683       | A           |
| 51         | A2           | 3685       | G           |
| 51         | A2           | 3700       | U           |
| 51         | A2           | 3707       | A           |
| 51         | A2           | 3717       | A           |
| 51         | A2           | 3718       | A           |
| 51         | A2           | 3724       | G           |
| 51         | A2           | 3726       | G           |
| 51         | A2           | 3731       | A           |
| 51         | A2           | 3732       | C           |
| 51         | A2           | 3747       | G           |
| 51         | A2           | 3748       | G           |
| 51         | A2           | 3749       | U           |
| 51         | A2           | 3751       | G           |
| 51         | A2           | 3754       | A           |
| 51         | A2           | 3781       | C           |
| 51         | A2           | 3782       | G           |
| 51         | A2           | 3783       | C           |
| 51         | A2           | 3784       | A           |
| 51         | A2           | 3788       | A           |
| 51         | A2           | 3789       | U           |
| 51         | A2           | 3790       | G           |
| 51         | A2           | 3795       | A           |
| 51         | A2           | 3798       | G           |
| 51         | A2           | 3799       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 3809       | U           |
| 51         | A2           | 3810       | G           |
| 51         | A2           | 3811       | U           |
| 51         | A2           | 3814       | C           |
| 51         | A2           | 3831       | A           |
| 51         | A2           | 3838       | A           |
| 51         | A2           | 3848       | A           |
| 51         | A2           | 3850       | G           |
| 51         | A2           | 3852       | G           |
| 51         | A2           | 3860       | G           |
| 51         | A2           | 3863       | U           |
| 51         | A2           | 3866       | G           |
| 51         | A2           | 3868       | G           |
| 51         | A2           | 3872       | A           |
| 51         | A2           | 3873       | A           |
| 51         | A2           | 3875       | G           |
| 51         | A2           | 3876       | A           |
| 51         | A2           | 3877       | A           |
| 51         | A2           | 3878       | G           |
| 51         | A2           | 3879       | A           |
| 51         | A2           | 3886       | U           |
| 51         | A2           | 3890       | C           |
| 51         | A2           | 3897       | C           |
| 51         | A2           | 3909       | G           |
| 51         | A2           | 3910       | G           |
| 51         | A2           | 3911       | U           |
| 51         | A2           | 3927       | G           |
| 51         | A2           | 3929       | G           |
| 51         | A2           | 3933       | A           |
| 51         | A2           | 3935       | U           |
| 51         | A2           | 3943       | A           |
| 51         | A2           | 3944       | G           |
| 51         | A2           | 4016       | A           |
| 51         | A2           | 4017       | A           |
| 51         | A2           | 4019       | U           |
| 51         | A2           | 4020       | A           |
| 51         | A2           | 4023       | A           |
| 51         | A2           | 4026       | A           |
| 51         | A2           | 4027       | C           |
| 51         | A2           | 4029       | C           |
| 51         | A2           | 4034       | C           |
| 51         | A2           | 4035       | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 4042       | C           |
| 51         | A2           | 4046       | G           |
| 51         | A2           | 4047       | A           |
| 51         | A2           | 4051       | G           |
| 51         | A2           | 4054       | G           |
| 51         | A2           | 4064       | G           |
| 51         | A2           | 4065       | G           |
| 51         | A2           | 4066       | C           |
| 51         | A2           | 4067       | G           |
| 51         | A2           | 4068       | A           |
| 51         | A2           | 4069       | G           |
| 51         | A2           | 4070       | C           |
| 51         | A2           | 4074       | A           |
| 51         | A2           | 4075       | G           |
| 51         | A2           | 4076       | G           |
| 51         | A2           | 4078       | G           |
| 51         | A2           | 4079       | C           |
| 51         | A2           | 4081       | C           |
| 51         | A2           | 4084       | G           |
| 51         | A2           | 4088       | C           |
| 51         | A2           | 4105       | C           |
| 51         | A2           | 4106       | C           |
| 51         | A2           | 4107       | C           |
| 51         | A2           | 4108       | G           |
| 51         | A2           | 4109       | G           |
| 51         | A2           | 4110       | C           |
| 51         | A2           | 4124       | C           |
| 51         | A2           | 4126       | C           |
| 51         | A2           | 4132       | A           |
| 51         | A2           | 4145       | G           |
| 51         | A2           | 4146       | G           |
| 51         | A2           | 4153       | G           |
| 51         | A2           | 4165       | A           |
| 51         | A2           | 4167       | A           |
| 51         | A2           | 4174       | A           |
| 51         | A2           | 4175       | A           |
| 51         | A2           | 4176       | A           |
| 51         | A2           | 4191       | U           |
| 51         | A2           | 4195       | A           |
| 51         | A2           | 4196       | A           |
| 51         | A2           | 4205       | C           |
| 51         | A2           | 4212       | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 4213       | A           |
| 51         | A2           | 4215       | A           |
| 51         | A2           | 4216       | G           |
| 51         | A2           | 4227       | U           |
| 51         | A2           | 4228       | G           |
| 51         | A2           | 4230       | A           |
| 51         | A2           | 4234       | G           |
| 51         | A2           | 4235       | A           |
| 51         | A2           | 4242       | A           |
| 51         | A2           | 4244       | A           |
| 51         | A2           | 4251       | U           |
| 51         | A2           | 4252       | U           |
| 51         | A2           | 4253       | G           |
| 51         | A2           | 4259       | G           |
| 51         | A2           | 4266       | A           |
| 51         | A2           | 4267       | G           |
| 51         | A2           | 4268       | U           |
| 51         | A2           | 4276       | C           |
| 51         | A2           | 4285       | A           |
| 51         | A2           | 4288       | G           |
| 51         | A2           | 4291       | G           |
| 51         | A2           | 4292       | G           |
| 51         | A2           | 4294       | C           |
| 51         | A2           | 4300       | G           |
| 51         | A2           | 4311       | C           |
| 51         | A2           | 4316       | U           |
| 51         | A2           | 4320       | U           |
| 51         | A2           | 4330       | G           |
| 51         | A2           | 4333       | G           |
| 51         | A2           | 4334       | U           |
| 51         | A2           | 4338       | A           |
| 51         | A2           | 4339       | G           |
| 51         | A2           | 4340       | A           |
| 51         | A2           | 4342       | A           |
| 51         | A2           | 4349       | C           |
| 51         | A2           | 4355       | G           |
| 51         | A2           | 4356       | A           |
| 51         | A2           | 4357       | U           |
| 51         | A2           | 4358       | A           |
| 51         | A2           | 4360       | C           |
| 51         | A2           | 4372       | G           |
| 51         | A2           | 4384       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 4388       | C           |
| 51         | A2           | 4392       | G           |
| 51         | A2           | 4406       | C           |
| 51         | A2           | 4410       | G           |
| 51         | A2           | 4412       | U           |
| 51         | A2           | 4426       | A           |
| 51         | A2           | 4427       | U           |
| 51         | A2           | 4428       | C           |
| 51         | A2           | 4437       | G           |
| 51         | A2           | 4455       | U           |
| 51         | A2           | 4459       | U           |
| 51         | A2           | 4474       | U           |
| 51         | A2           | 4475       | A           |
| 51         | A2           | 4477       | G           |
| 51         | A2           | 4480       | A           |
| 51         | A2           | 4482       | G           |
| 51         | A2           | 4485       | A           |
| 51         | A2           | 4486       | G           |
| 51         | A2           | 4510       | A           |
| 51         | A2           | 4522       | C           |
| 51         | A2           | 4532       | G           |
| 51         | A2           | 4537       | G           |
| 51         | A2           | 4543       | G           |
| 51         | A2           | 4551       | A           |
| 51         | A2           | 4552       | A           |
| 51         | A2           | 4561       | A           |
| 51         | A2           | 4562       | G           |
| 51         | A2           | 4568       | G           |
| 51         | A2           | 4579       | G           |
| 51         | A2           | 4586       | A           |
| 51         | A2           | 4595       | G           |
| 51         | A2           | 4598       | U           |
| 51         | A2           | 4599       | G           |
| 51         | A2           | 4614       | G           |
| 51         | A2           | 4618       | A           |
| 51         | A2           | 4620       | G           |
| 51         | A2           | 4632       | C           |
| 51         | A2           | 4633       | C           |
| 51         | A2           | 4640       | G           |
| 51         | A2           | 4641       | G           |
| 51         | A2           | 4649       | A           |
| 51         | A2           | 4655       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 4656       | G           |
| 51         | A2           | 4662       | A           |
| 51         | A2           | 4665       | U           |
| 51         | A2           | 4671       | U           |
| 51         | A2           | 4678       | C           |
| 51         | A2           | 4680       | G           |
| 51         | A2           | 4681       | G           |
| 51         | A2           | 4693       | G           |
| 51         | A2           | 4694       | G           |
| 51         | A2           | 4695       | C           |
| 51         | A2           | 4696       | A           |
| 51         | A2           | 4700       | C           |
| 51         | A2           | 4703       | C           |
| 51         | A2           | 4704       | G           |
| 51         | A2           | 4705       | G           |
| 51         | A2           | 4713       | G           |
| 51         | A2           | 4714       | U           |
| 51         | A2           | 4715       | U           |
| 51         | A2           | 4718       | C           |
| 51         | A2           | 4720       | U           |
| 51         | A2           | 4725       | U           |
| 51         | A2           | 4726       | A           |
| 51         | A2           | 4731       | G           |
| 51         | A2           | 4732       | U           |
| 51         | A2           | 4824       | C           |
| 51         | A2           | 4827       | U           |
| 51         | A2           | 4828       | G           |
| 51         | A2           | 4831       | G           |
| 51         | A2           | 4832       | A           |
| 51         | A2           | 4833       | G           |
| 51         | A2           | 4834       | U           |
| 51         | A2           | 4837       | C           |
| 51         | A2           | 4838       | C           |
| 51         | A2           | 4839       | U           |
| 51         | A2           | 4840       | U           |
| 51         | A2           | 4841       | C           |
| 51         | A2           | 4847       | G           |
| 51         | A2           | 4852       | A           |
| 51         | A2           | 4853       | C           |
| 51         | A2           | 4854       | G           |
| 51         | A2           | 4855       | G           |
| 51         | A2           | 4856       | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 4858       | C           |
| 51         | A2           | 4859       | G           |
| 51         | A2           | 4860       | C           |
| 51         | A2           | 4864       | C           |
| 51         | A2           | 4865       | G           |
| 51         | A2           | 4866       | G           |
| 51         | A2           | 4867       | A           |
| 51         | A2           | 4868       | A           |
| 51         | A2           | 4869       | A           |
| 51         | A2           | 4870       | G           |
| 51         | A2           | 4871       | G           |
| 51         | A2           | 4872       | C           |
| 51         | A2           | 4880       | C           |
| 51         | A2           | 4882       | C           |
| 51         | A2           | 4883       | U           |
| 51         | A2           | 4885       | G           |
| 51         | A2           | 4886       | C           |
| 51         | A2           | 4895       | C           |
| 51         | A2           | 4896       | A           |
| 51         | A2           | 4899       | G           |
| 51         | A2           | 4901       | A           |
| 51         | A2           | 4902       | C           |
| 51         | A2           | 4905       | U           |
| 51         | A2           | 4906       | C           |
| 51         | A2           | 4907       | G           |
| 51         | A2           | 4908       | U           |
| 51         | A2           | 4909       | G           |
| 51         | A2           | 4921       | G           |
| 51         | A2           | 4924       | A           |
| 51         | A2           | 4934       | U           |
| 51         | A2           | 4936       | G           |
| 51         | A2           | 4943       | U           |
| 51         | A2           | 4946       | U           |
| 51         | A2           | 4947       | U           |
| 51         | A2           | 4948       | C           |
| 51         | A2           | 4949       | U           |
| 51         | A2           | 4950       | G           |
| 51         | A2           | 4957       | G           |
| 51         | A2           | 4960       | U           |
| 51         | A2           | 4964       | U           |
| 51         | A2           | 4971       | C           |
| 51         | A2           | 4972       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | A2           | 4975       | G           |
| 51         | A2           | 4981       | C           |
| 51         | A2           | 4982       | C           |
| 51         | A2           | 4984       | U           |
| 51         | A2           | 4985       | C           |
| 51         | A2           | 4986       | G           |
| 51         | A2           | 4998       | U           |
| 51         | A2           | 4999       | G           |
| 51         | A2           | 5005       | C           |
| 51         | A2           | 5008       | C           |
| 51         | A2           | 5011       | U           |
| 51         | A2           | 5012       | C           |
| 51         | A2           | 5013       | G           |
| 51         | A2           | 5016       | A           |
| 51         | A2           | 5019       | A           |
| 51         | A2           | 5020       | G           |
| 51         | A2           | 5024       | U           |
| 51         | A2           | 5028       | C           |
| 52         | B1           | 4          | C           |
| 52         | B1           | 17         | C           |
| 52         | B1           | 25         | A           |
| 52         | B1           | 26         | U           |
| 52         | B1           | 33         | G           |
| 52         | B1           | 46         | A           |
| 52         | B1           | 59         | U           |
| 52         | B1           | 66         | G           |
| 52         | B1           | 67         | C           |
| 52         | B1           | 72         | C           |
| 52         | B1           | 73         | C           |
| 52         | B1           | 74         | G           |
| 52         | B1           | 77         | A           |
| 52         | B1           | 79         | A           |
| 52         | B1           | 85         | A           |
| 52         | B1           | 91         | A           |
| 52         | B1           | 103        | A           |
| 52         | B1           | 107        | A           |
| 52         | B1           | 110        | U           |
| 52         | B1           | 113        | G           |
| 52         | B1           | 114        | G           |
| 52         | B1           | 115        | U           |
| 52         | B1           | 125        | C           |
| 52         | B1           | 126        | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 52         | B1           | 142        | C           |
| 52         | B1           | 143        | U           |
| 52         | B1           | 146        | G           |
| 52         | B1           | 153        | G           |
| 52         | B1           | 155        | G           |
| 52         | B1           | 159        | A           |
| 52         | B1           | 160        | U           |
| 52         | B1           | 161        | U           |
| 52         | B1           | 162        | C           |
| 52         | B1           | 163        | U           |
| 52         | B1           | 170        | A           |
| 52         | B1           | 172        | U           |
| 52         | B1           | 173        | A           |
| 52         | B1           | 174        | C           |
| 52         | B1           | 175        | A           |
| 52         | B1           | 183        | G           |
| 52         | B1           | 188        | C           |
| 52         | B1           | 192        | C           |
| 52         | B1           | 202        | G           |
| 52         | B1           | 217        | A           |
| 52         | B1           | 219        | U           |
| 52         | B1           | 225        | G           |
| 52         | B1           | 226        | A           |
| 52         | B1           | 227        | U           |
| 52         | B1           | 228        | C           |
| 52         | B1           | 229        | A           |
| 52         | B1           | 230        | A           |
| 52         | B1           | 238        | C           |
| 52         | B1           | 239        | C           |
| 52         | B1           | 283        | G           |
| 52         | B1           | 284        | C           |
| 52         | B1           | 285        | U           |
| 52         | B1           | 286        | U           |
| 52         | B1           | 287        | U           |
| 52         | B1           | 292        | A           |
| 52         | B1           | 293        | C           |
| 52         | B1           | 298        | G           |
| 52         | B1           | 302        | A           |
| 52         | B1           | 306        | C           |
| 52         | B1           | 308        | G           |
| 52         | B1           | 309        | G           |
| 52         | B1           | 313        | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 52         | B1           | 314        | U           |
| 52         | B1           | 319        | C           |
| 52         | B1           | 325        | C           |
| 52         | B1           | 327        | G           |
| 52         | B1           | 328        | U           |
| 52         | B1           | 329        | G           |
| 52         | B1           | 331        | C           |
| 52         | B1           | 332        | G           |
| 52         | B1           | 333        | G           |
| 52         | B1           | 339        | A           |
| 52         | B1           | 343        | A           |
| 52         | B1           | 347        | G           |
| 52         | B1           | 351        | G           |
| 52         | B1           | 357        | C           |
| 52         | B1           | 362        | C           |
| 52         | B1           | 364        | A           |
| 52         | B1           | 368        | U           |
| 52         | B1           | 369        | C           |
| 52         | B1           | 370        | G           |
| 52         | B1           | 376        | A           |
| 52         | B1           | 381        | C           |
| 52         | B1           | 385        | G           |
| 52         | B1           | 386        | C           |
| 52         | B1           | 387        | C           |
| 52         | B1           | 398        | A           |
| 52         | B1           | 408        | A           |
| 52         | B1           | 409        | C           |
| 52         | B1           | 426        | A           |
| 52         | B1           | 427        | U           |
| 52         | B1           | 435        | A           |
| 52         | B1           | 447        | A           |
| 52         | B1           | 448        | A           |
| 52         | B1           | 449        | A           |
| 52         | B1           | 450        | C           |
| 52         | B1           | 463        | C           |
| 52         | B1           | 464        | A           |
| 52         | B1           | 465        | A           |
| 52         | B1           | 467        | G           |
| 52         | B1           | 471        | G           |
| 52         | B1           | 472        | C           |
| 52         | B1           | 474        | G           |
| 52         | B1           | 476        | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 52         | B1           | 482        | G           |
| 52         | B1           | 483        | C           |
| 52         | B1           | 485        | A           |
| 52         | B1           | 487        | U           |
| 52         | B1           | 489        | A           |
| 52         | B1           | 492        | C           |
| 52         | B1           | 493        | A           |
| 52         | B1           | 496        | C           |
| 52         | B1           | 501        | C           |
| 52         | B1           | 503        | C           |
| 52         | B1           | 508        | A           |
| 52         | B1           | 517        | C           |
| 52         | B1           | 523        | A           |
| 52         | B1           | 525        | A           |
| 52         | B1           | 526        | A           |
| 52         | B1           | 527        | C           |
| 52         | B1           | 529        | A           |
| 52         | B1           | 533        | A           |
| 52         | B1           | 534        | G           |
| 52         | B1           | 535        | G           |
| 52         | B1           | 536        | A           |
| 52         | B1           | 541        | U           |
| 52         | B1           | 542        | U           |
| 52         | B1           | 544        | G           |
| 52         | B1           | 545        | A           |
| 52         | B1           | 546        | G           |
| 52         | B1           | 547        | G           |
| 52         | B1           | 548        | C           |
| 52         | B1           | 549        | C           |
| 52         | B1           | 550        | C           |
| 52         | B1           | 553        | U           |
| 52         | B1           | 554        | A           |
| 52         | B1           | 555        | A           |
| 52         | B1           | 558        | G           |
| 52         | B1           | 560        | A           |
| 52         | B1           | 562        | U           |
| 52         | B1           | 565        | G           |
| 52         | B1           | 567        | C           |
| 52         | B1           | 587        | A           |
| 52         | B1           | 589        | G           |
| 52         | B1           | 590        | A           |
| 52         | B1           | 591        | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 52         | B1           | 592        | C           |
| 52         | B1           | 597        | G           |
| 52         | B1           | 606        | G           |
| 52         | B1           | 607        | U           |
| 52         | B1           | 608        | C           |
| 52         | B1           | 613        | G           |
| 52         | B1           | 614        | C           |
| 52         | B1           | 617        | G           |
| 52         | B1           | 620        | G           |
| 52         | B1           | 621        | C           |
| 52         | B1           | 623        | G           |
| 52         | B1           | 629        | A           |
| 52         | B1           | 634        | A           |
| 52         | B1           | 643        | A           |
| 52         | B1           | 644        | G           |
| 52         | B1           | 645        | C           |
| 52         | B1           | 657        | U           |
| 52         | B1           | 658        | U           |
| 52         | B1           | 660        | C           |
| 52         | B1           | 662        | G           |
| 52         | B1           | 668        | A           |
| 52         | B1           | 669        | A           |
| 52         | B1           | 672        | A           |
| 52         | B1           | 673        | G           |
| 52         | B1           | 684        | G           |
| 52         | B1           | 688        | U           |
| 52         | B1           | 690        | G           |
| 52         | B1           | 741        | C           |
| 52         | B1           | 742        | U           |
| 52         | B1           | 743        | U           |
| 52         | B1           | 744        | G           |
| 52         | B1           | 747        | U           |
| 52         | B1           | 751        | G           |
| 52         | B1           | 791        | C           |
| 52         | B1           | 796        | G           |
| 52         | B1           | 797        | C           |
| 52         | B1           | 798        | G           |
| 52         | B1           | 799        | U           |
| 52         | B1           | 800        | U           |
| 52         | B1           | 806        | U           |
| 52         | B1           | 808        | A           |
| 52         | B1           | 810        | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 52         | B1           | 811        | A           |
| 52         | B1           | 821        | G           |
| 52         | B1           | 827        | A           |
| 52         | B1           | 836        | G           |
| 52         | B1           | 837        | A           |
| 52         | B1           | 839        | C           |
| 52         | B1           | 841        | G           |
| 52         | B1           | 847        | A           |
| 52         | B1           | 848        | U           |
| 52         | B1           | 868        | G           |
| 52         | B1           | 870        | A           |
| 52         | B1           | 871        | U           |
| 52         | B1           | 874        | G           |
| 52         | B1           | 885        | U           |
| 52         | B1           | 888        | U           |
| 52         | B1           | 890        | U           |
| 52         | B1           | 891        | G           |
| 52         | B1           | 913        | A           |
| 52         | B1           | 914        | U           |
| 52         | B1           | 917        | U           |
| 52         | B1           | 919        | A           |
| 52         | B1           | 920        | A           |
| 52         | B1           | 928        | G           |
| 52         | B1           | 929        | G           |
| 52         | B1           | 933        | G           |
| 52         | B1           | 943        | U           |
| 52         | B1           | 950        | C           |
| 52         | B1           | 955        | A           |
| 52         | B1           | 956        | G           |
| 52         | B1           | 958        | G           |
| 52         | B1           | 959        | G           |
| 52         | B1           | 960        | U           |
| 52         | B1           | 962        | A           |
| 52         | B1           | 963        | A           |
| 52         | B1           | 969        | U           |
| 52         | B1           | 975        | G           |
| 52         | B1           | 988        | C           |
| 52         | B1           | 990        | A           |
| 52         | B1           | 991        | G           |
| 52         | B1           | 992        | A           |
| 52         | B1           | 1002       | U           |
| 52         | B1           | 1008       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 52         | B1           | 1017       | U           |
| 52         | B1           | 1021       | U           |
| 52         | B1           | 1023       | A           |
| 52         | B1           | 1044       | G           |
| 52         | B1           | 1053       | C           |
| 52         | B1           | 1057       | C           |
| 52         | B1           | 1060       | A           |
| 52         | B1           | 1061       | U           |
| 52         | B1           | 1062       | A           |
| 52         | B1           | 1076       | G           |
| 52         | B1           | 1077       | A           |
| 52         | B1           | 1085       | C           |
| 52         | B1           | 1088       | U           |
| 52         | B1           | 1100       | A           |
| 52         | B1           | 1109       | C           |
| 52         | B1           | 1110       | G           |
| 52         | B1           | 1113       | A           |
| 52         | B1           | 1114       | U           |
| 52         | B1           | 1115       | U           |
| 52         | B1           | 1116       | C           |
| 52         | B1           | 1117       | C           |
| 52         | B1           | 1119       | A           |
| 52         | B1           | 1120       | U           |
| 52         | B1           | 1121       | G           |
| 52         | B1           | 1123       | C           |
| 52         | B1           | 1133       | A           |
| 52         | B1           | 1140       | G           |
| 52         | B1           | 1146       | C           |
| 52         | B1           | 1149       | A           |
| 52         | B1           | 1150       | A           |
| 52         | B1           | 1156       | U           |
| 52         | B1           | 1157       | G           |
| 52         | B1           | 1163       | C           |
| 52         | B1           | 1170       | A           |
| 52         | B1           | 1195       | A           |
| 52         | B1           | 1199       | A           |
| 52         | B1           | 1203       | G           |
| 52         | B1           | 1207       | G           |
| 52         | B1           | 1215       | C           |
| 52         | B1           | 1224       | G           |
| 52         | B1           | 1242       | U           |
| 52         | B1           | 1251       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 52         | B1           | 1253       | A           |
| 52         | B1           | 1256       | G           |
| 52         | B1           | 1257       | G           |
| 52         | B1           | 1258       | A           |
| 52         | B1           | 1259       | A           |
| 52         | B1           | 1261       | C           |
| 52         | B1           | 1271       | C           |
| 52         | B1           | 1275       | G           |
| 52         | B1           | 1276       | A           |
| 52         | B1           | 1285       | G           |
| 52         | B1           | 1286       | G           |
| 52         | B1           | 1287       | A           |
| 52         | B1           | 1288       | U           |
| 52         | B1           | 1289       | U           |
| 52         | B1           | 1290       | G           |
| 52         | B1           | 1297       | U           |
| 52         | B1           | 1301       | A           |
| 52         | B1           | 1302       | G           |
| 52         | B1           | 1303       | C           |
| 52         | B1           | 1312       | G           |
| 52         | B1           | 1313       | A           |
| 52         | B1           | 1314       | U           |
| 52         | B1           | 1320       | G           |
| 52         | B1           | 1330       | G           |
| 52         | B1           | 1331       | C           |
| 52         | B1           | 1332       | A           |
| 52         | B1           | 1342       | U           |
| 52         | B1           | 1352       | G           |
| 52         | B1           | 1371       | U           |
| 52         | B1           | 1372       | U           |
| 52         | B1           | 1373       | C           |
| 52         | B1           | 1378       | A           |
| 52         | B1           | 1381       | G           |
| 52         | B1           | 1382       | A           |
| 52         | B1           | 1394       | G           |
| 52         | B1           | 1397       | U           |
| 52         | B1           | 1398       | G           |
| 52         | B1           | 1399       | C           |
| 52         | B1           | 1401       | A           |
| 52         | B1           | 1406       | G           |
| 52         | B1           | 1417       | C           |
| 52         | B1           | 1418       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 52         | B1           | 1420       | G           |
| 52         | B1           | 1421       | A           |
| 52         | B1           | 1424       | G           |
| 52         | B1           | 1426       | U           |
| 52         | B1           | 1439       | A           |
| 52         | B1           | 1442       | U           |
| 52         | B1           | 1444       | U           |
| 52         | B1           | 1454       | A           |
| 52         | B1           | 1455       | A           |
| 52         | B1           | 1461       | G           |
| 52         | B1           | 1462       | U           |
| 52         | B1           | 1463       | U           |
| 52         | B1           | 1477       | U           |
| 52         | B1           | 1478       | U           |
| 52         | B1           | 1480       | A           |
| 52         | B1           | 1484       | A           |
| 52         | B1           | 1489       | A           |
| 52         | B1           | 1494       | U           |
| 52         | B1           | 1495       | G           |
| 52         | B1           | 1497       | G           |
| 52         | B1           | 1498       | A           |
| 52         | B1           | 1507       | G           |
| 52         | B1           | 1512       | C           |
| 52         | B1           | 1519       | U           |
| 52         | B1           | 1520       | G           |
| 52         | B1           | 1521       | C           |
| 52         | B1           | 1522       | A           |
| 52         | B1           | 1531       | A           |
| 52         | B1           | 1533       | A           |
| 52         | B1           | 1537       | A           |
| 52         | B1           | 1544       | C           |
| 52         | B1           | 1548       | G           |
| 52         | B1           | 1553       | C           |
| 52         | B1           | 1554       | C           |
| 52         | B1           | 1555       | U           |
| 52         | B1           | 1558       | C           |
| 52         | B1           | 1560       | U           |
| 52         | B1           | 1573       | G           |
| 52         | B1           | 1580       | A           |
| 52         | B1           | 1582       | C           |
| 52         | B1           | 1584       | G           |
| 52         | B1           | 1585       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 52         | B1           | 1586       | U           |
| 52         | B1           | 1587       | G           |
| 52         | B1           | 1588       | A           |
| 52         | B1           | 1601       | A           |
| 52         | B1           | 1604       | G           |
| 52         | B1           | 1606       | G           |
| 52         | B1           | 1618       | C           |
| 52         | B1           | 1620       | A           |
| 52         | B1           | 1621       | U           |
| 52         | B1           | 1622       | U           |
| 52         | B1           | 1623       | A           |
| 52         | B1           | 1624       | U           |
| 52         | B1           | 1660       | C           |
| 52         | B1           | 1661       | A           |
| 52         | B1           | 1662       | U           |
| 52         | B1           | 1663       | A           |
| 52         | B1           | 1665       | G           |
| 52         | B1           | 1671       | G           |
| 52         | B1           | 1678       | A           |
| 52         | B1           | 1695       | A           |
| 52         | B1           | 1699       | A           |
| 52         | B1           | 1703       | C           |
| 52         | B1           | 1721       | U           |
| 52         | B1           | 1722       | G           |
| 52         | B1           | 1737       | G           |
| 52         | B1           | 1756       | C           |
| 52         | B1           | 1757       | G           |
| 52         | B1           | 1776       | G           |
| 52         | B1           | 1779       | G           |
| 52         | B1           | 1782       | G           |
| 52         | B1           | 1783       | C           |
| 52         | B1           | 1784       | G           |
| 52         | B1           | 1801       | A           |
| 52         | B1           | 1811       | C           |
| 52         | B1           | 1823       | A           |
| 52         | B1           | 1829       | G           |
| 52         | B1           | 1834       | A           |
| 52         | B1           | 1838       | U           |
| 52         | B1           | 1849       | G           |
| 52         | B1           | 1851       | A           |
| 52         | B1           | 1852       | C           |
| 52         | B1           | 1860       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 52         | B1           | 1861       | G           |
| 52         | B1           | 1862       | G           |
| 52         | B1           | 1863       | A           |
| 52         | B1           | 1865       | C           |
| 52         | B1           | 1866       | A           |
| 52         | B1           | 1869       | A           |
| 83         | Bv           | 4          | C           |
| 83         | Bv           | 7          | A           |
| 83         | Bv           | 8          | U           |
| 83         | Bv           | 11         | C           |
| 83         | Bv           | 13         | C           |
| 83         | Bv           | 14         | A           |
| 83         | Bv           | 16         | U           |
| 83         | Bv           | 17         | C           |
| 83         | Bv           | 18         | G           |
| 83         | Bv           | 19         | G           |
| 83         | Bv           | 30         | G           |
| 83         | Bv           | 37         | A           |
| 83         | Bv           | 43         | C           |
| 83         | Bv           | 46         | G           |
| 83         | Bv           | 48         | C           |
| 83         | Bv           | 53         | G           |
| 83         | Bv           | 56         | C           |
| 83         | Bv           | 58         | A           |
| 83         | Bv           | 59         | U           |
| 83         | Bv           | 61         | C           |
| 83         | Bv           | 68         | C           |
| 83         | Bv           | 75         | C           |
| 83         | Bv           | 76         | A           |
| 84         | Bx           | 45         | U           |
| 84         | Bx           | 46         | U           |
| 84         | Bx           | 49         | U           |
| 84         | Bx           | 50         | U           |
| 84         | Bx           | 51         | U           |
| 84         | Bx           | 53         | U           |
| 84         | Bx           | 54         | U           |
| 84         | Bx           | 56         | U           |
| 84         | Bx           | 57         | U           |
| 84         | Bx           | 58         | U           |

All (28) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A3    | 33   | G    |
| 7   | A3    | 39   | G    |
| 7   | A3    | 108  | A    |
| 51  | A2    | 31   | U    |
| 51  | A2    | 71   | C    |
| 51  | A2    | 227  | G    |
| 51  | A2    | 228  | U    |
| 51  | A2    | 901  | U    |
| 51  | A2    | 959  | C    |
| 51  | A2    | 1500 | A    |
| 51  | A2    | 2717 | C    |
| 51  | A2    | 3755 | A    |
| 51  | A2    | 4107 | C    |
| 51  | A2    | 4661 | U    |
| 51  | A2    | 4865 | G    |
| 51  | A2    | 4870 | G    |
| 51  | A2    | 4907 | G    |
| 51  | A2    | 4946 | U    |
| 52  | B1    | 173  | A    |
| 52  | B1    | 227  | U    |
| 52  | B1    | 286  | U    |
| 52  | B1    | 369  | C    |
| 52  | B1    | 644  | G    |
| 52  | B1    | 797  | C    |
| 52  | B1    | 1139 | C    |
| 52  | B1    | 1398 | G    |
| 52  | B1    | 1554 | C    |
| 52  | B1    | 1756 | C    |

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

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

#### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

Of 332 ligands modelled in this entry, 331 are monoatomic - leaving 1 for Mogul analysis.



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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 88  | MVM  | A2    | 5327 | -    | 33,35,35     | 1.77 | 4 (12%)  | 36,49,49    | 2.23 | 13 (36%) |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 88  | MVM  | A2    | 5327 | -    | -       | 0/20/28/28 | 0/5/5/5 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 88  | A2    | 5327 | MVM  | C5-N1  | 6.48  | 1.46        | 1.37     |
| 88  | A2    | 5327 | MVM  | N5-N4  | -4.44 | 1.30        | 1.37     |
| 88  | A2    | 5327 | MVM  | C6-N1  | 2.57  | 1.45        | 1.39     |
| 88  | A2    | 5327 | MVM  | C12-C5 | 2.45  | 1.54        | 1.50     |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 88  | A2    | 5327 | MVM  | C15-N4-C22 | -5.43 | 124.12      | 129.98   |
| 88  | A2    | 5327 | MVM  | C21-N7-C22 | 4.68  | 122.58      | 116.77   |
| 88  | A2    | 5327 | MVM  | C7-C3-C9   | 4.33  | 119.43      | 110.82   |
| 88  | A2    | 5327 | MVM  | N3-C6-N1   | 3.81  | 120.36      | 116.33   |
| 88  | A2    | 5327 | MVM  | C1-C9-N1   | -3.69 | 106.90      | 116.16   |
| 88  | A2    | 5327 | MVM  | C19-C18-N6 | 3.42  | 135.76      | 130.19   |
| 88  | A2    | 5327 | MVM  | C12-C5-N1  | 3.31  | 122.79      | 118.40   |
| 88  | A2    | 5327 | MVM  | C15-N4-N5  | 3.18  | 125.04      | 119.95   |
| 88  | A2    | 5327 | MVM  | C8-N3-C6   | 2.88  | 121.82      | 115.14   |
| 88  | A2    | 5327 | MVM  | N6-N5-N4   | 2.70  | 109.38      | 106.37   |
| 88  | A2    | 5327 | MVM  | C20-C21-N7 | -2.64 | 119.90      | 123.94   |
| 88  | A2    | 5327 | MVM  | C11-C2-C6  | 2.29  | 120.83      | 118.54   |
| 88  | A2    | 5327 | MVM  | C2-C6-N3   | -2.09 | 119.54      | 122.91   |

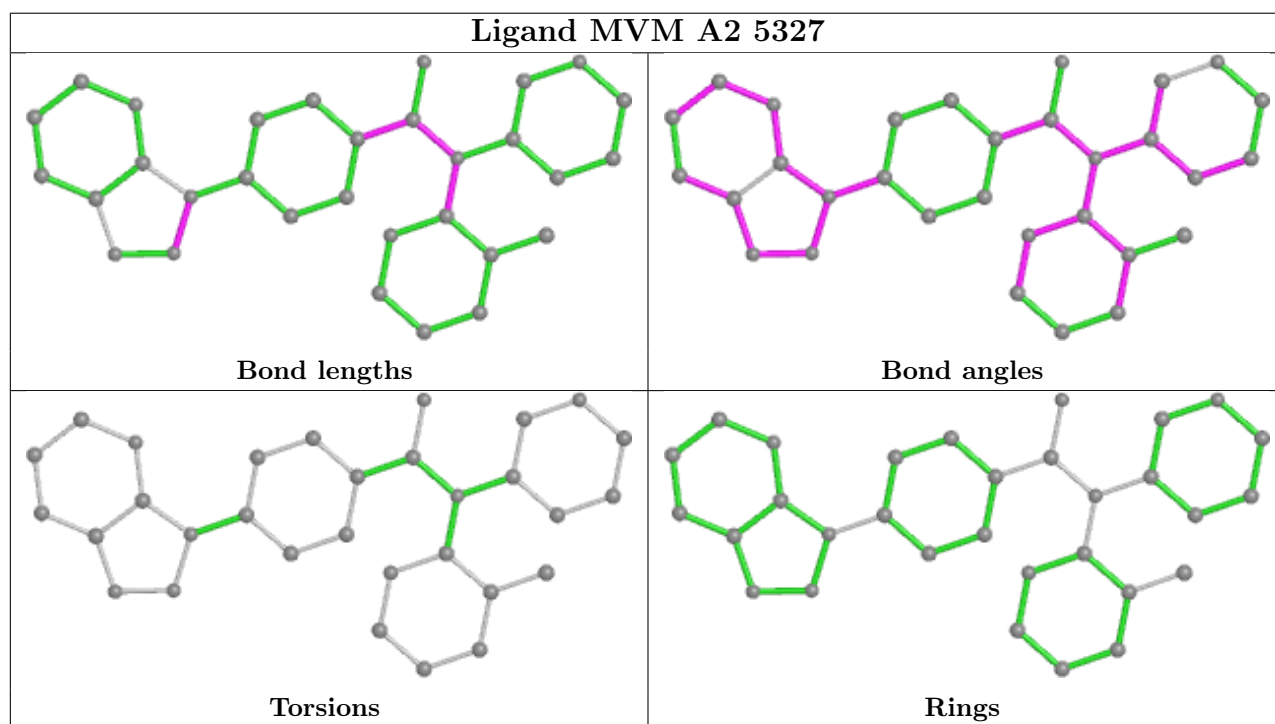
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 51  | A2    | 11               |
| 52  | B1    | 6                |
| 83  | Bv    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B1    | 126:G     | O3'    | 141:A     | P      | 20.56        |
| 1     | B1    | 1757:G    | O3'    | 1775:U    | P      | 18.28        |
| 1     | A2    | 3948:C    | O3'    | 4004:G    | P      | 18.11        |
| 1     | B1    | 751:G     | O3'    | 790:C     | P      | 17.98        |
| 1     | A2    | 4734:C    | O3'    | 4818:G    | P      | 17.83        |
| 1     | A2    | 750:G     | O3'    | 890:C     | P      | 17.39        |
| 1     | A2    | 1680:C    | O3'    | 1699:C    | P      | 17.31        |
| 1     | B1    | 1426:U    | O3'    | 1438:A    | P      | 17.22        |
| 1     | A2    | 1233:C    | O3'    | 1243:G    | P      | 17.05        |
| 1     | A2    | 517:C     | O3'    | 629:G     | P      | 17.01        |
| 1     | B1    | 240:G     | O3'    | 282:G     | P      | 16.73        |
| 1     | A2    | 2881:G    | O3'    | 3569:C    | P      | 16.22        |
| 1     | A2    | 976:U     | O3'    | 1047:G    | P      | 15.81        |
| 1     | A2    | 1089:A    | O3'    | 1145:G    | P      | 15.47        |
| 1     | B1    | 696:G     | O3'    | 737:G     | P      | 15.40        |
| 1     | A2    | 2068:C    | O3'    | 2245:C    | P      | 14.47        |
| 1     | A2    | 1202:G    | O3'    | 1216:G    | P      | 13.43        |
| 1     | Bv    | 73:A      | O3'    | 74:C      | P      | 1.78         |

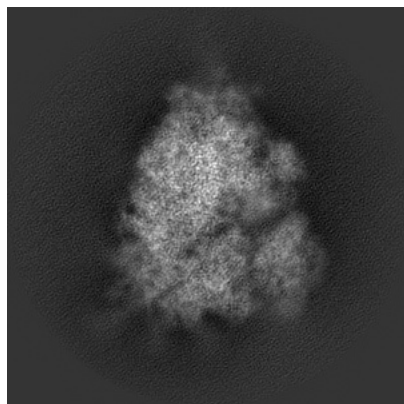
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0601. These allow visual inspection of the internal detail of the map and identification of artifacts.

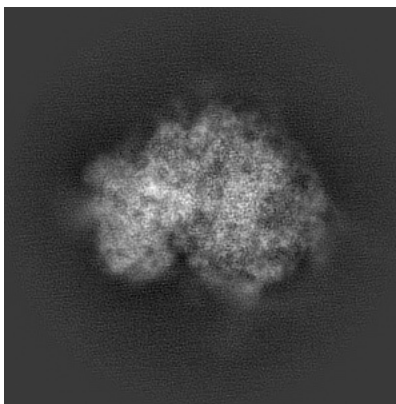
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

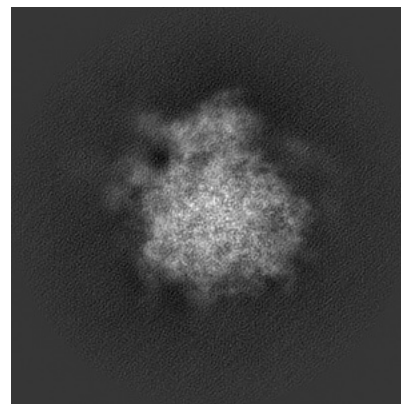
#### 6.1.1 Primary map



X

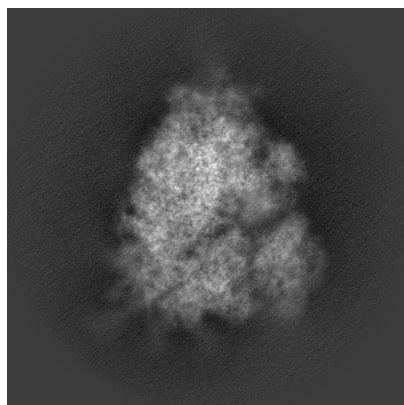


Y

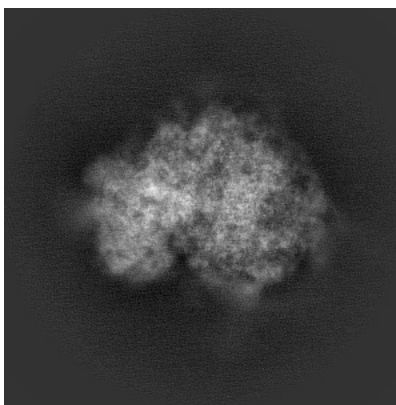


Z

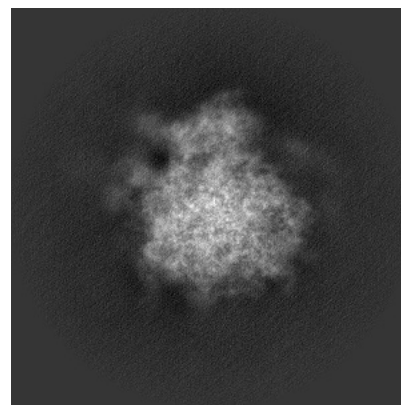
#### 6.1.2 Raw map



X



Y

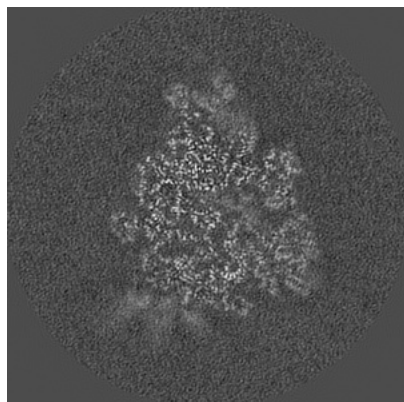


Z

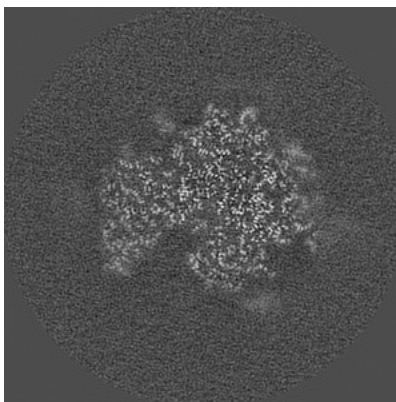
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

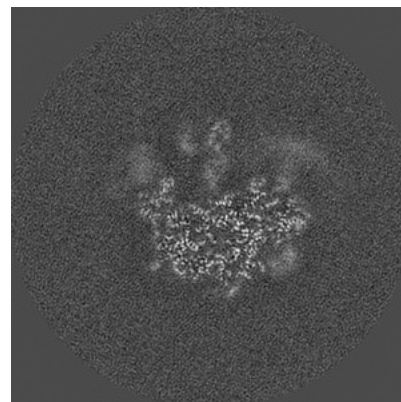
### 6.2.1 Primary map



X Index: 205

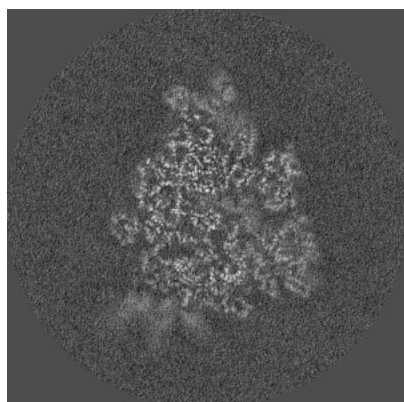


Y Index: 205

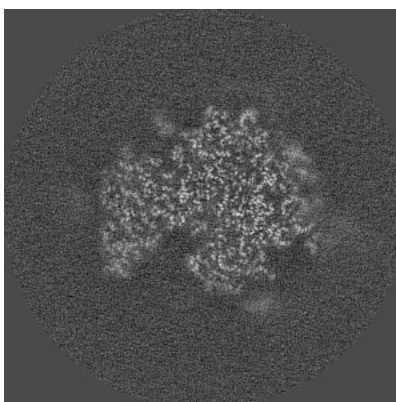


Z Index: 205

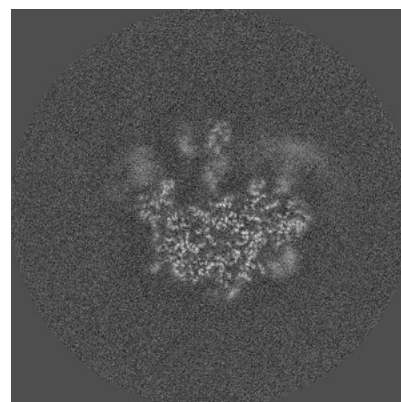
### 6.2.2 Raw map



X Index: 205



Y Index: 205



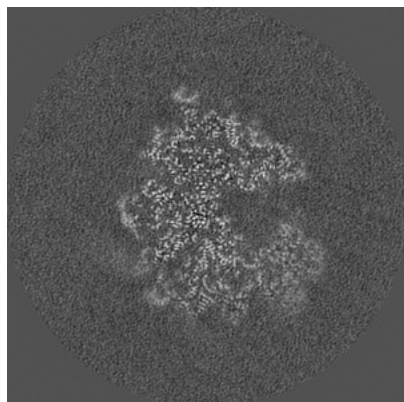
Z Index: 205

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

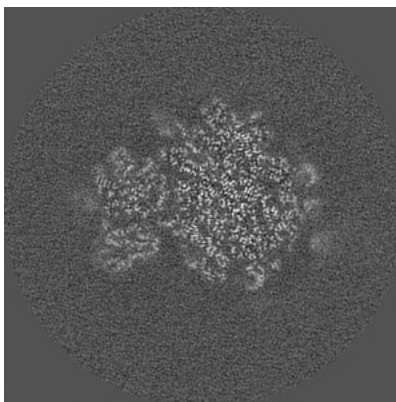


## 6.3 Largest variance slices [i](#)

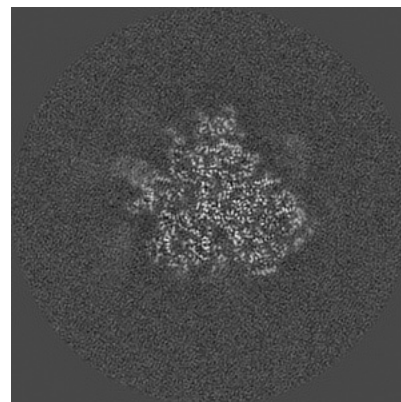
### 6.3.1 Primary map



X Index: 225

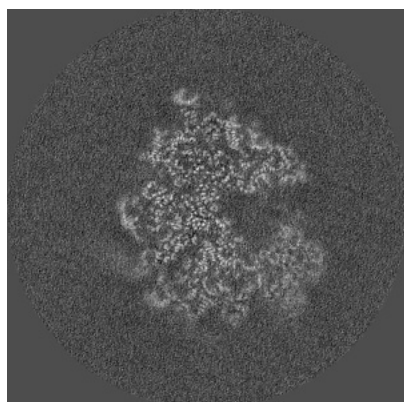


Y Index: 197

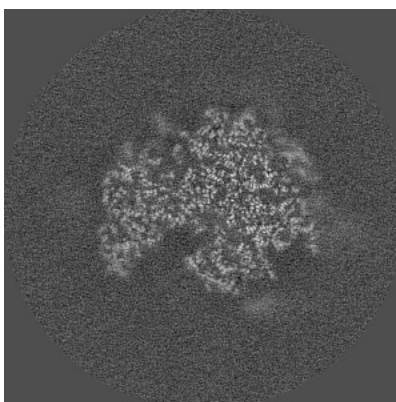


Z Index: 234

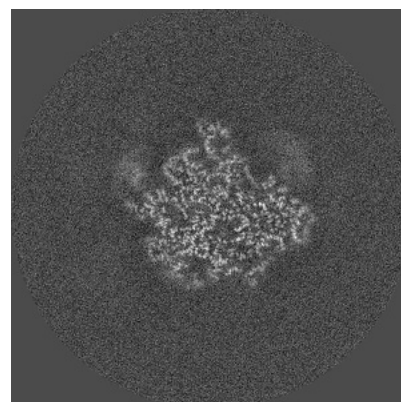
### 6.3.2 Raw map



X Index: 225



Y Index: 207

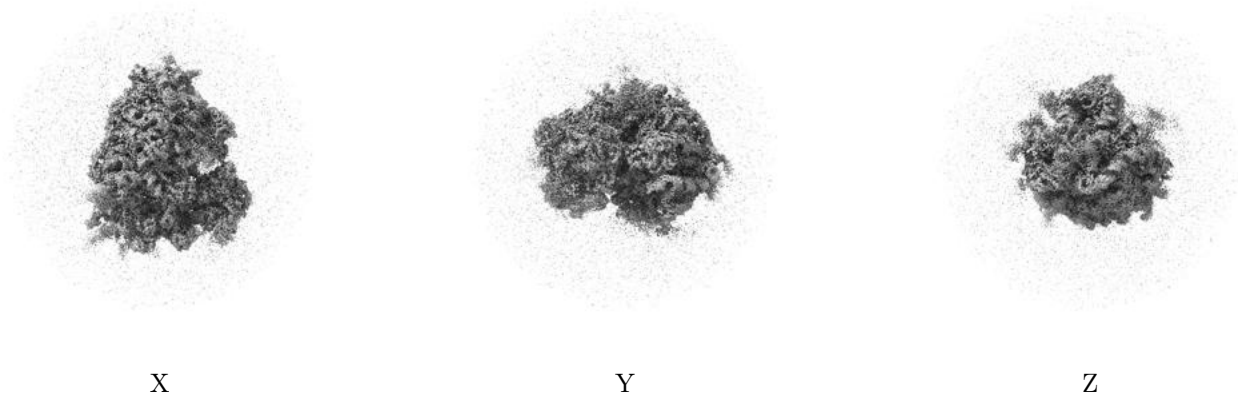


Z Index: 225

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

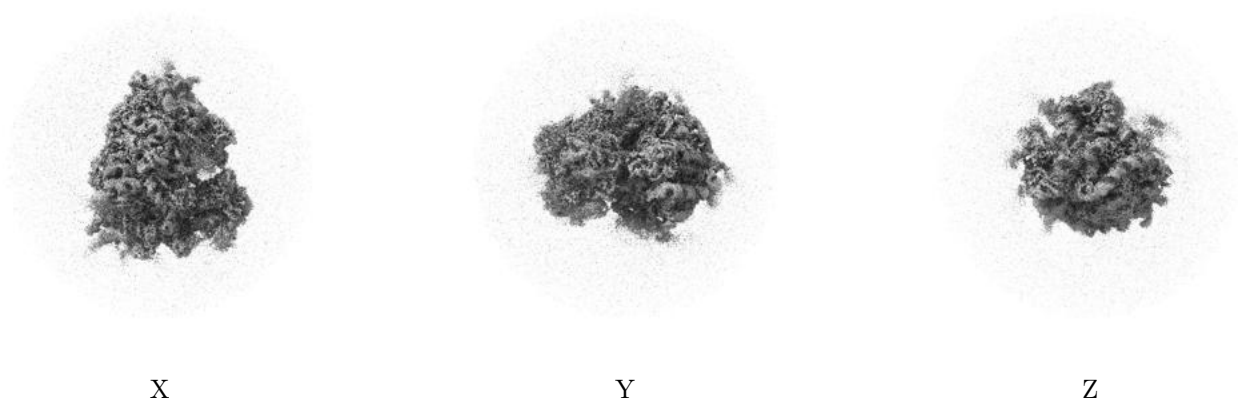
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

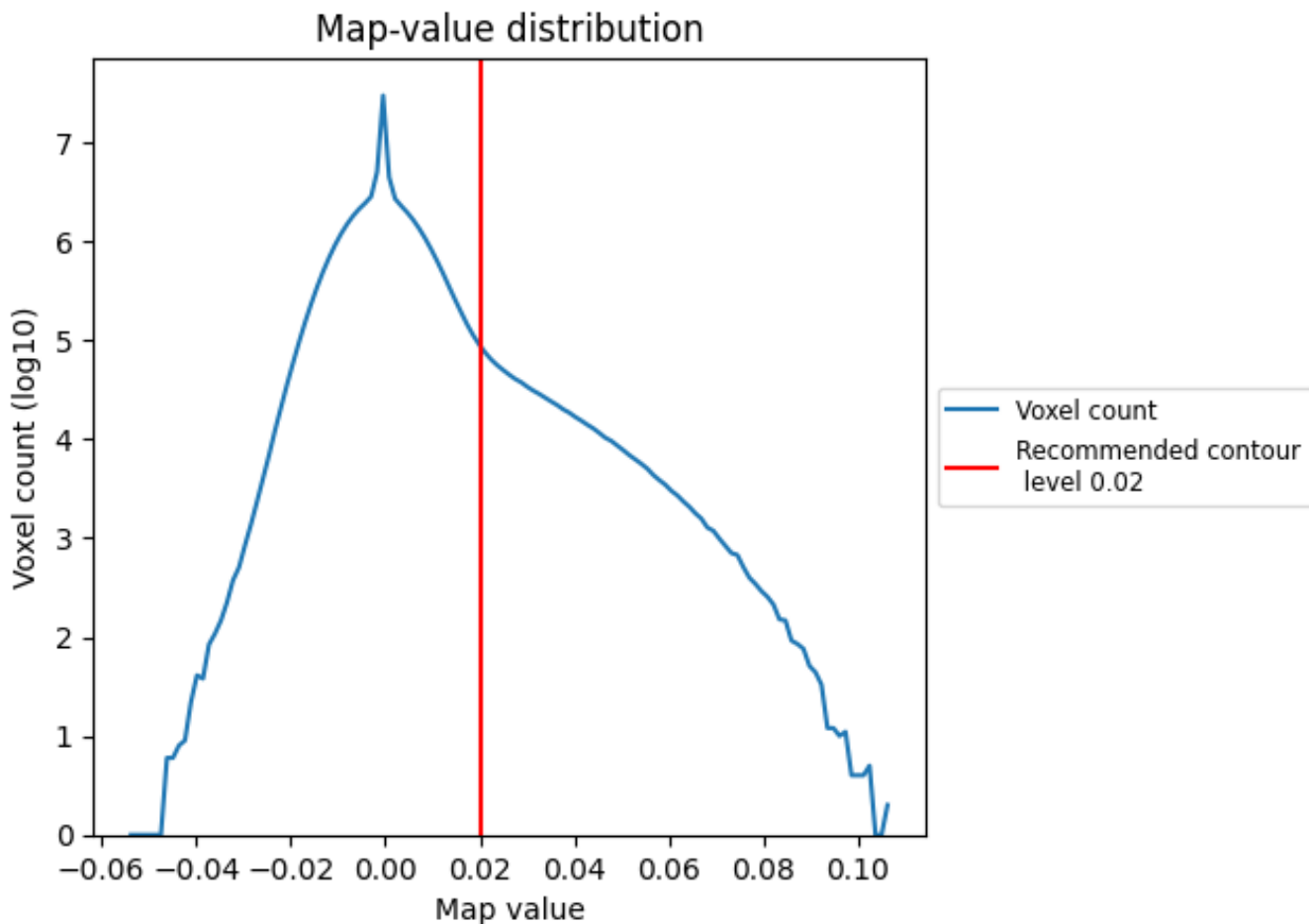
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

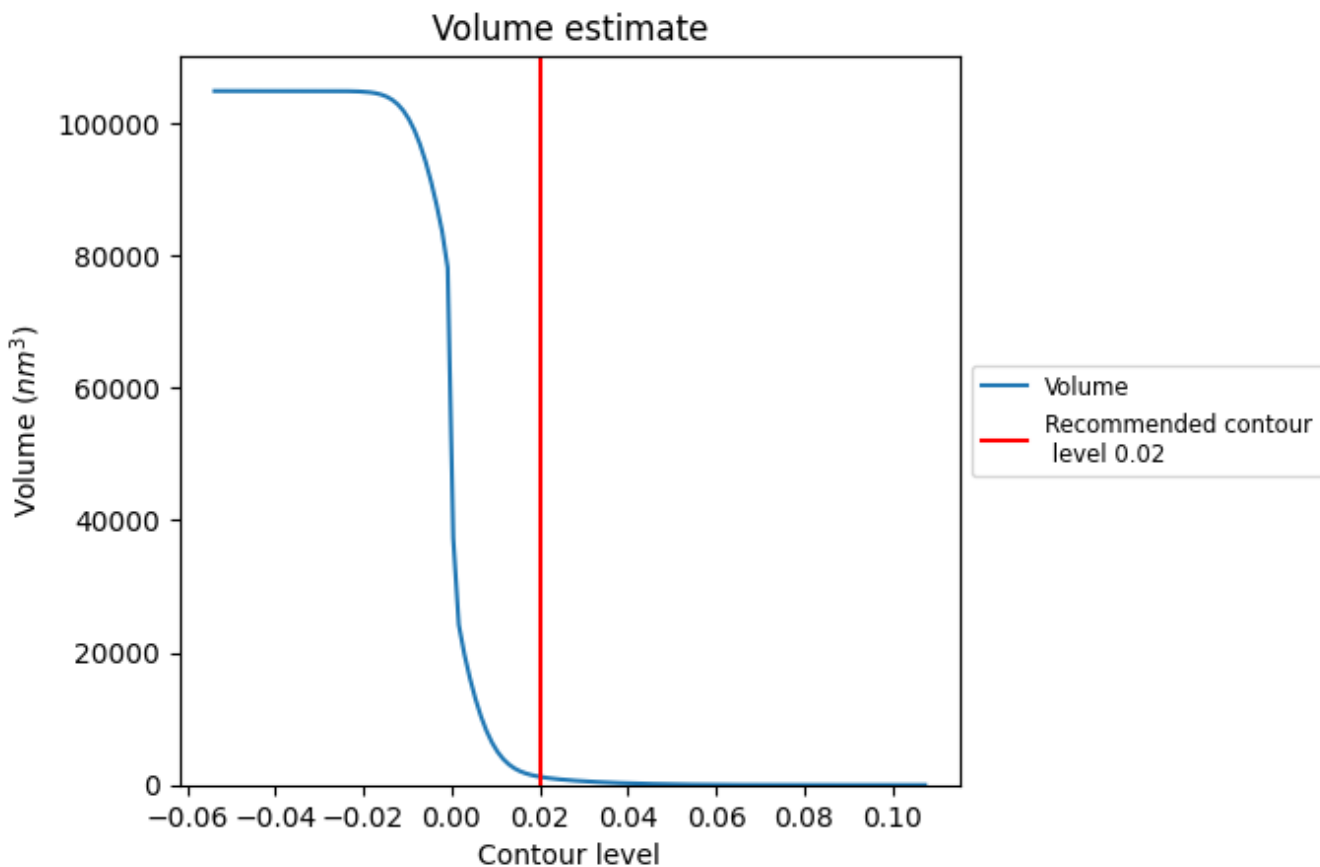
### 7.1 Map-value distribution [i](#)



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



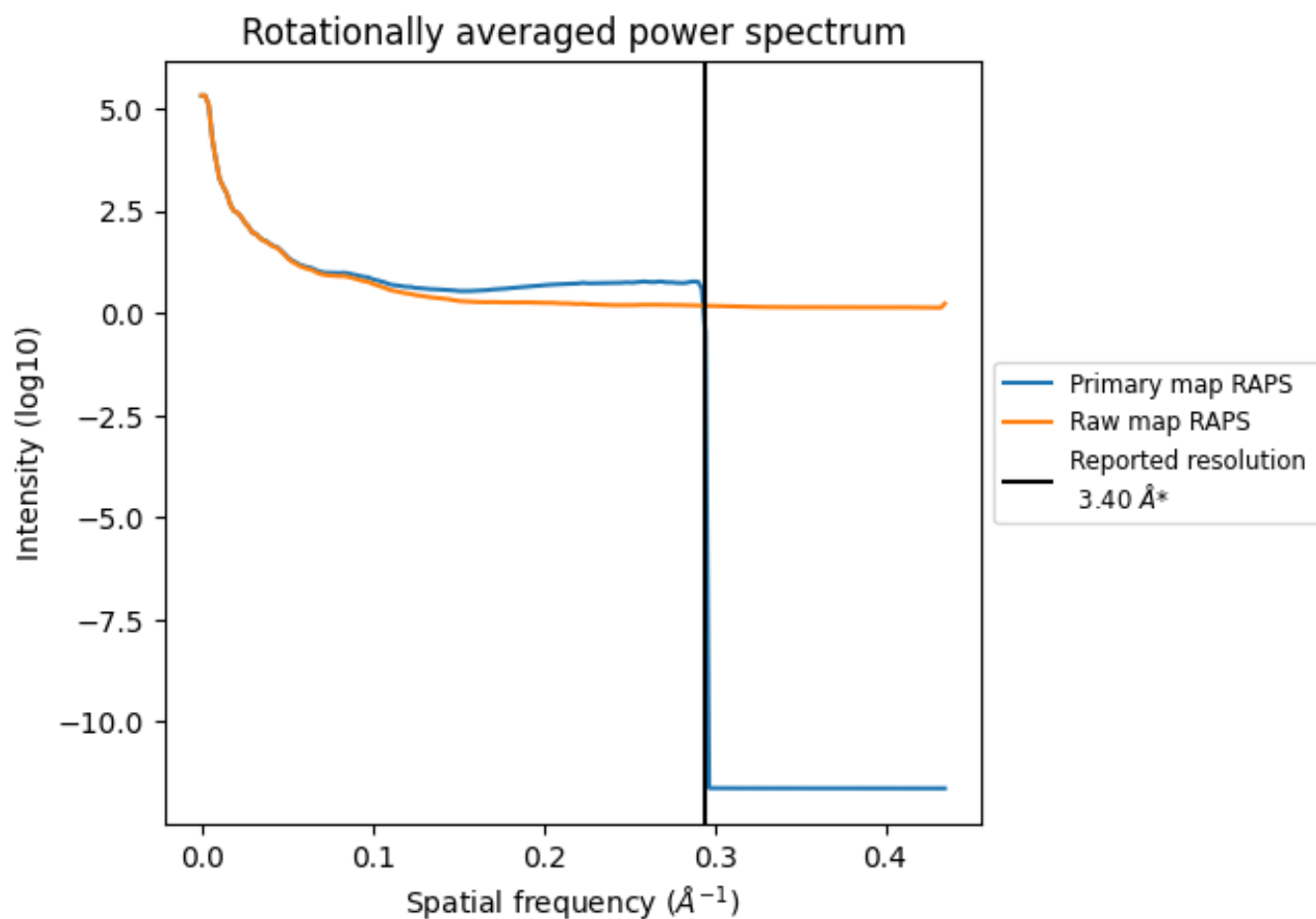
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1242 nm<sup>3</sup>; this corresponds to an approximate mass of 1122 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 [i](#)

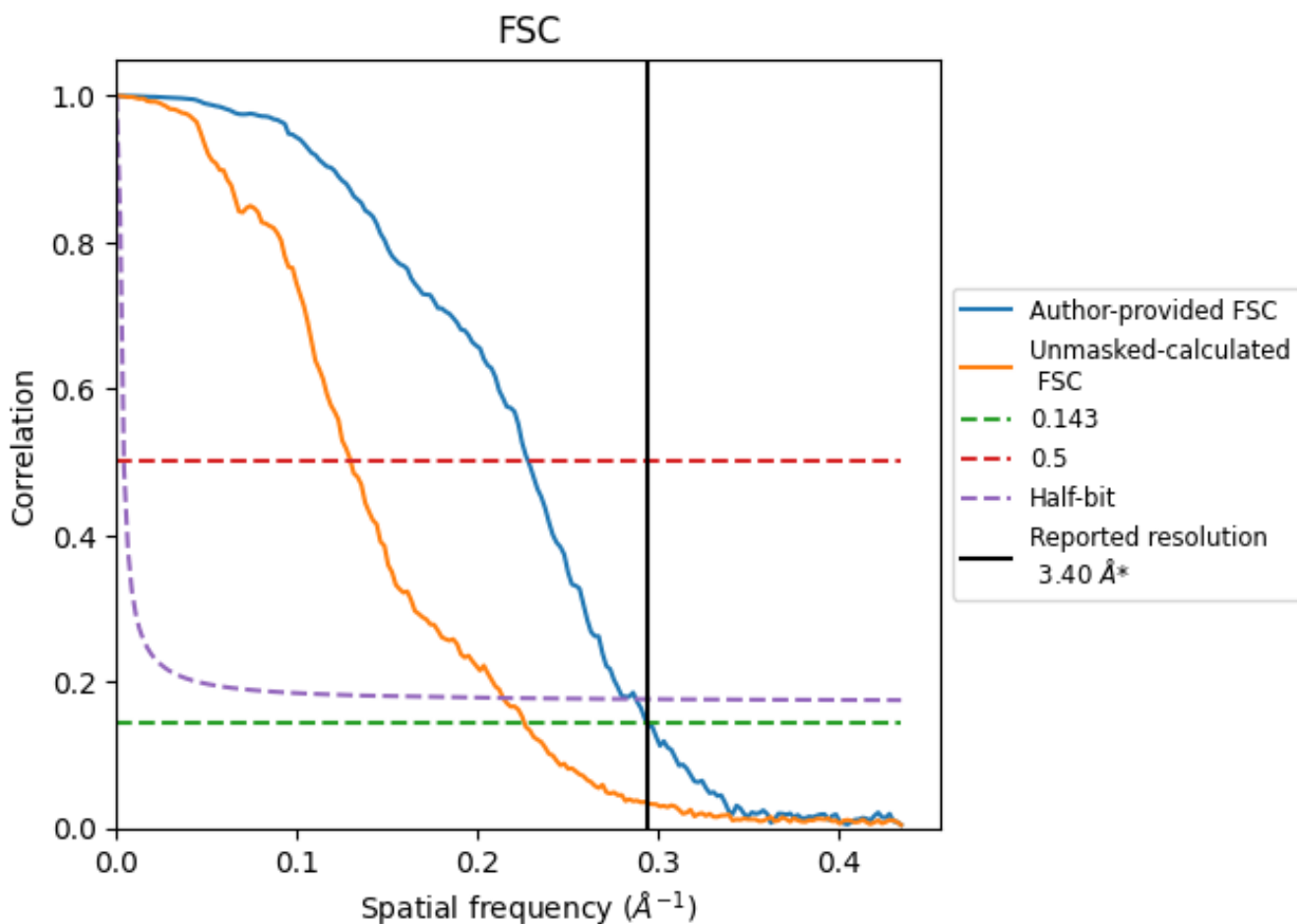


\*Reported resolution corresponds to spatial frequency of  $0.294 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

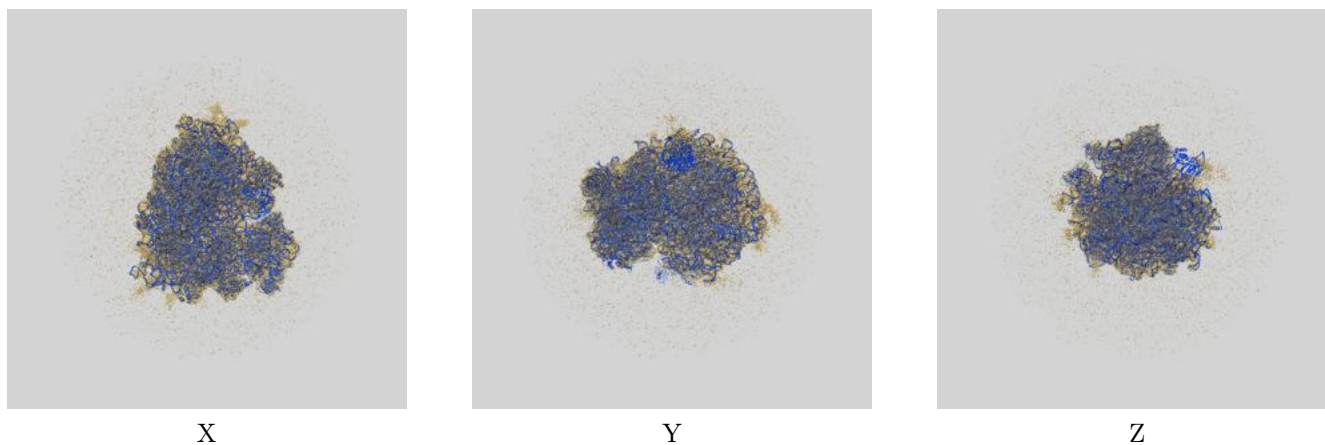
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.40                               | -    | -        |
| Author-provided FSC curve | 3.40                               | 4.38 | 3.47     |
| Unmasked-calculated*      | 4.42                               | 7.70 | 4.67     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.42 differs from the reported value 3.4 by more than 10 %

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

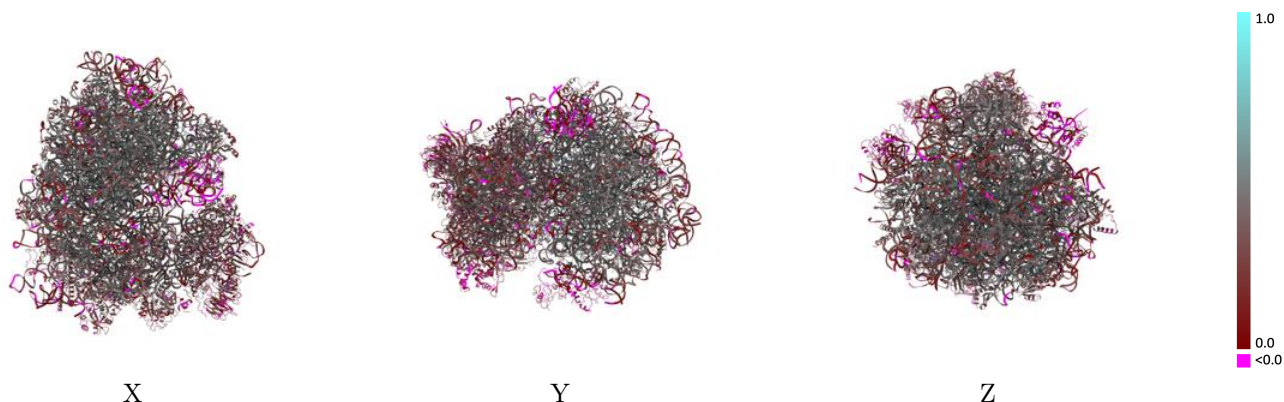
This section contains information regarding the fit between EMDB map EMD-0601 and PDB model 6OLG. Per-residue inclusion information can be found in section 3 on page 21.

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



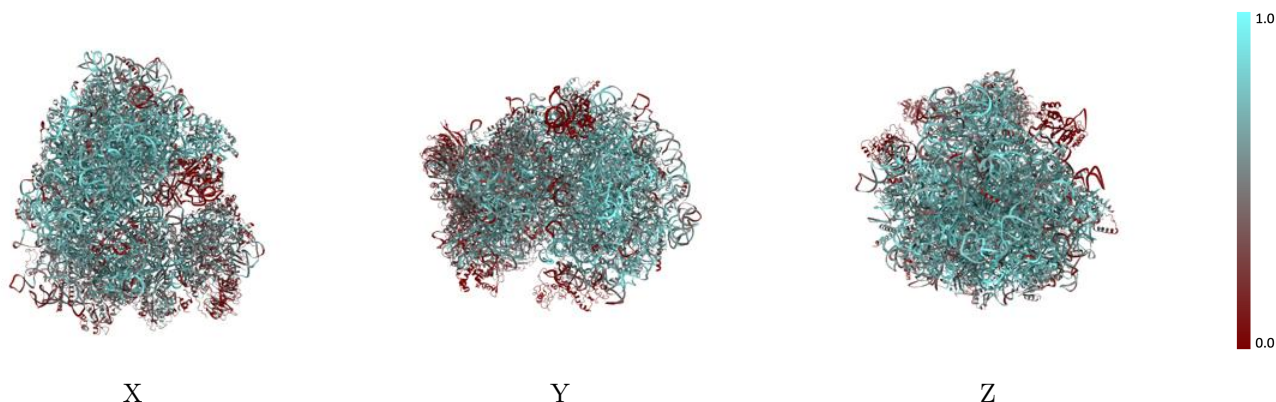
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



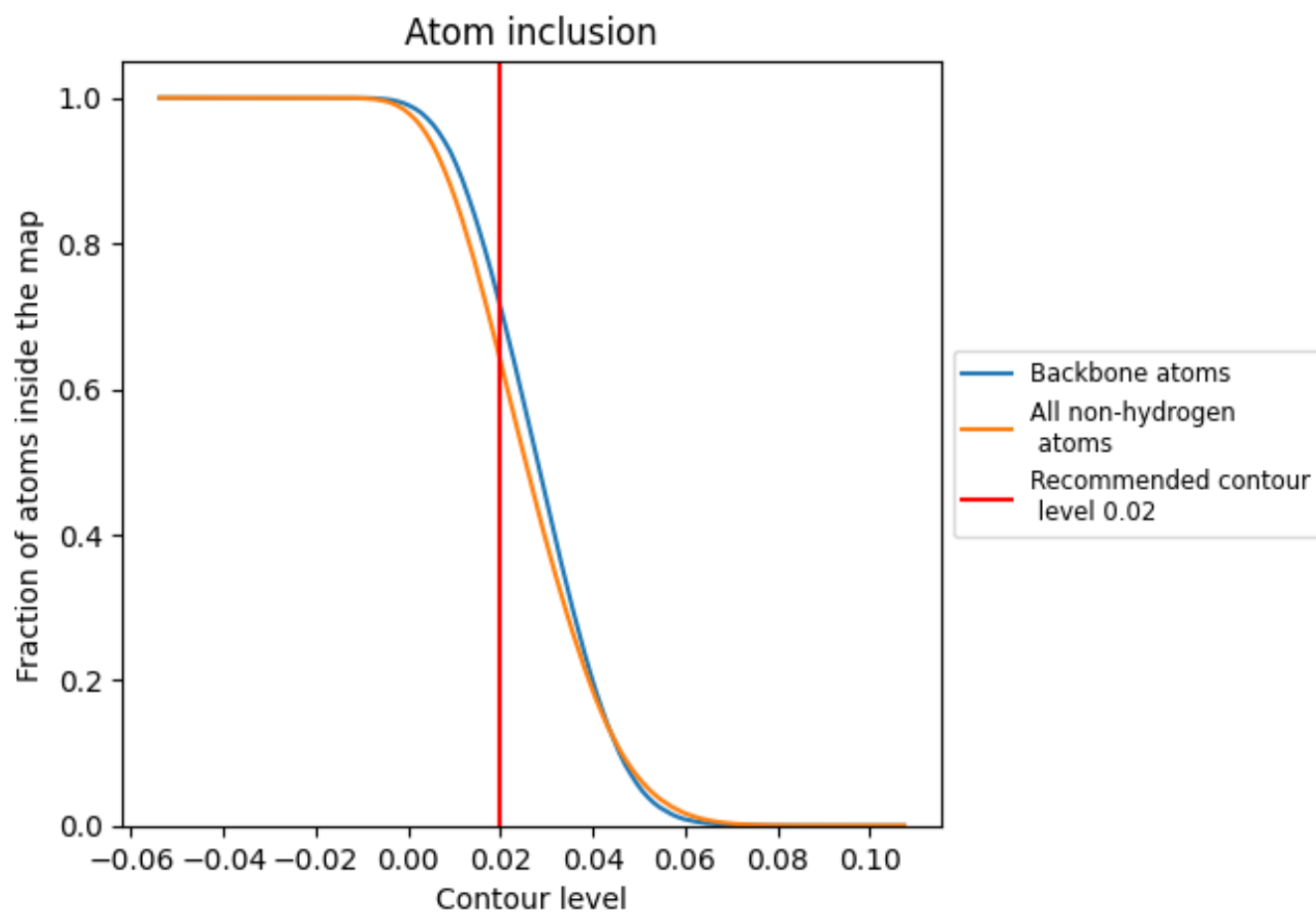
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 64% 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 (0.02) and Q-score for the entire model and for each chain.





















































































| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.6387   |  0.3630   |
| A     |  0.0737   |  0.0390   |
| A2    |  0.7525   |  0.3930   |
| A3    |  0.7643   |  0.3980   |
| A4    |  0.8627   |  0.4520   |
| AA    |  0.6722   |  0.4320   |
| AB    |  0.6504   |  0.4280   |
| AC    |  0.6682   |  0.4320   |
| AD    |  0.6232   |  0.3830   |
| AE    |  0.5414   |  0.3590   |
| AF    |  0.6378   |  0.4090   |
| AG    |  0.5641   |  0.3510   |
| AH    |  0.5733   |  0.3930   |
| AI    |  0.6195   |  0.4030   |
| AJ    |  0.5678  |  0.3670  |
| AK    |  0.0387 |  0.0470 |
| AL    |  0.5950 |  0.3720 |
| AM    |  0.6477 |  0.4040 |
| AN    |  0.7228 |  0.4480 |
| AO    |  0.6527 |  0.4190 |
| AP    |  0.6603 |  0.4370 |
| AQ    |  0.6485 |  0.4270 |
| AR    |  0.6269 |  0.3870 |
| AS    |  0.6736 |  0.4430 |
| AT    |  0.6589 |  0.4100 |
| AU    |  0.5418 |  0.3530 |
| AV    |  0.6484 |  0.4400 |
| AW    |  0.3732 |  0.2640 |
| AX    |  0.6004 |  0.4040 |
| AY    |  0.6605 |  0.4130 |
| AZ    |  0.6230 |  0.3660 |
| Aa    |  0.6950 |  0.4390 |
| Ab    |  0.5875 |  0.3580 |
| Ac    |  0.5816 |  0.3890 |
| Ad    |  0.6392 |  0.4050 |



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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| Ae    |  0.6816   |  0.4450   |
| Af    |  0.7043   |  0.4620   |
| Ag    |  0.6203   |  0.4080   |
| Ah    |  0.6065   |  0.3720   |
| Ai    |  0.6194   |  0.3560   |
| Aj    |  0.7169   |  0.4510   |
| Ak    |  0.5045   |  0.3110   |
| Al    |  0.6548   |  0.4200   |
| Am    |  0.6448   |  0.4080   |
| An    |  0.5525   |  0.3670   |
| Ao    |  0.5716   |  0.3850   |
| Ap    |  0.6531   |  0.4230   |
| Aq    |  0.0205   |  0.0630   |
| At    |  0.6652   |  0.4220   |
| Au    |  0.0064   |  0.0330   |
| B1    |  0.6887   |  0.3570   |
| BA    |  0.5003   |  0.3260   |
| BB    |  0.4858  |  0.3100  |
| BC    |  0.5443 |  0.3690 |
| BD    |  0.3343 |  0.2720 |
| BE    |  0.5126 |  0.3530 |
| BF    |  0.4073 |  0.2760 |
| BG    |  0.3955 |  0.2560 |
| BH    |  0.3738 |  0.2540 |
| BI    |  0.5098 |  0.3430 |
| BJ    |  0.5031 |  0.3120 |
| BK    |  0.2783 |  0.2000 |
| BL    |  0.5168 |  0.3390 |
| BM    |  0.0414 |  0.0730 |
| BN    |  0.5377 |  0.3460 |
| BO    |  0.5329 |  0.3590 |
| BP    |  0.3713 |  0.2340 |
| BQ    |  0.4110 |  0.2550 |
| BR    |  0.3540 |  0.2520 |
| BS    |  0.3933 |  0.2800 |
| BT    |  0.3688 |  0.2290 |
| BU    |  0.3720 |  0.2510 |
| BV    |  0.4859 |  0.3190 |
| BW    |  0.5832 |  0.3830 |
| BX    |  0.5611 |  0.3700 |
| BY    |  0.4569 |  0.2880 |
| BZ    |  0.3065 |  0.2130 |

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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| Ba    |  0.5609 |  0.3270 |
| Bb    |  0.4551 |  0.3050 |
| Bc    |  0.3660 |  0.2660 |
| Bd    |  0.4537 |  0.3030 |
| Be    |  0.4123 |  0.2940 |
| Bf    |  0.0925 |  0.1090 |
| Bg    |  0.2134 |  0.1920 |
| Bv    |  0.3692 |  0.2530 |
| Bx    |  0.0906 |  0.0900 |