



## Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 07:11 AM EDT

PDB ID : 4V71 / pdb\_00004v71  
EMDB ID : EMD-1717  
Title : E. coli 70S-fMetVal-tRNAVal-tRNA<sup>f</sup>Met complex in intermediate pre-translocation state (pre2)  
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.  
Deposited on : 2013-10-14  
Resolution : 20.00 Å (reported)  
Based on initial models : 2HGP, 2WRI, 3I1O, 2K4C

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:

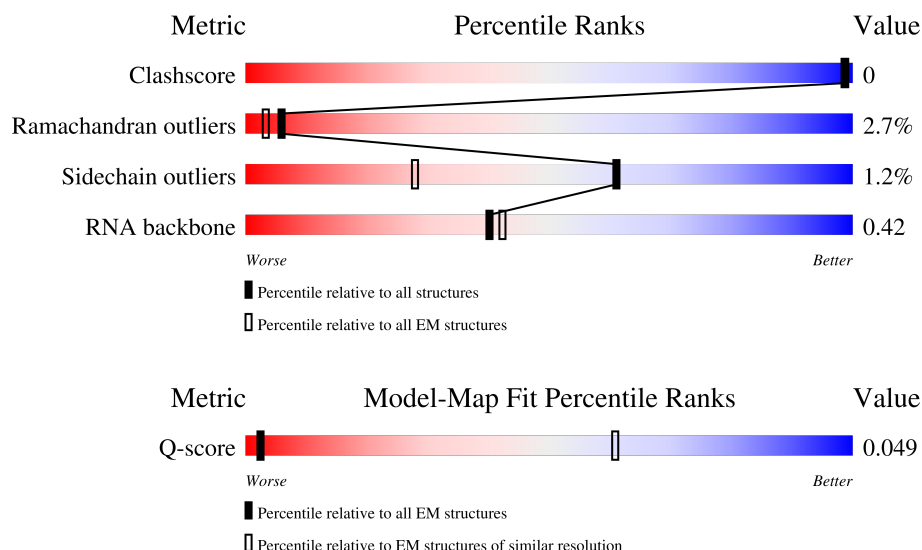
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 20.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 28 ( 19.50 - 20.50 )                                     |

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   | AB    | 220    | <div> <div>56%</div> <div>97%</div> <div>•</div> </div>  |
| 2   | AC    | 208    | <div> <div>36%</div> <div>97%</div> <div>•</div> </div>  |
| 3   | AD    | 206    | <div> <div>49%</div> <div>95%</div> <div>5%</div> </div> |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--------------------|
| 4   | AE    | 152    | 16% 95% ..         |
| 5   | AF    | 101    | 28% 96% .          |
| 6   | AG    | 152    | 53% 97% ..         |
| 7   | AH    | 130    | 22% 93% 6% .       |
| 8   | AI    | 128    | 36% 95% 5% .       |
| 9   | AJ    | 100    | 38% 91% 7% .       |
| 10  | AK    | 118    | 36% 92% 8% .       |
| 11  | AL    | 124    | 44% 94% . ..       |
| 12  | AM    | 115    | 26% 94% 5% .       |
| 13  | AN    | 101    | 33% 97% ..         |
| 14  | AO    | 89     | 24% 93% 6% .       |
| 15  | AP    | 81     | 36% 96% .          |
| 16  | AQ    | 82     | 39% 96% .          |
| 17  | AR    | 57     | 44% 95% . .        |
| 18  | AS    | 81     | 26% 94% 5% .       |
| 19  | AT    | 86     | 16% 94% 5% .       |
| 20  | AU    | 53     | 49% 87% 11% .      |
| 21  | AA    | 1533   | 8% 60% 32% 7% .    |
| 22  | A1    | 76     | 50% 49% 42% 8% .   |
| 23  | A2    | 15     | 33% 47% 33% 7% 13% |
| 24  | A3    | 77     | 22% 62% 27% 10%    |
| 25  | BC    | 273    | 53% 94% 6%         |
| 26  | BD    | 209    | 36% 92% 8%         |
| 27  | BE    | 201    | 31% 95% 5%         |
| 28  | BF    | 179    | 21% 93% 6% .       |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | BG    | 177    |                  |
| 30  | BH    | 149    |                  |
| 31  | BI    | 142    |                  |
| 32  | BJ    | 142    |                  |
| 33  | BK    | 123    |                  |
| 34  | BL    | 144    |                  |
| 35  | BM    | 136    |                  |
| 36  | BN    | 121    |                  |
| 37  | BO    | 117    |                  |
| 38  | BP    | 115    |                  |
| 39  | BQ    | 118    |                  |
| 40  | BR    | 103    |                  |
| 41  | BS    | 110    |                  |
| 42  | BT    | 94     |                  |
| 43  | BU    | 104    |                  |
| 44  | BV    | 94     |                  |
| 45  | BW    | 80     |                  |
| 46  | BX    | 79     |                  |
| 47  | BY    | 63     |                  |
| 48  | BZ    | 59     |                  |
| 49  | B0    | 57     |                  |
| 50  | B1    | 52     |                  |
| 51  | B2    | 46     |                  |
| 52  | B3    | 65     |                  |
| 53  | B4    | 38     |                  |

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| Mol | Chain | Length | Quality of chain                                                                         |
|-----|-------|--------|------------------------------------------------------------------------------------------|
| 54  | BA    | 2903   | <div><div></div><div>16%</div><div>60%</div><div>32%</div><div>7%</div><div></div></div> |
| 55  | BB    | 118    | <div><div></div><div>10%</div><div>68%</div><div>28%</div><div></div><div></div></div>   |
| 56  | B5    | 234    | <div><div></div><div>76%</div><div>93%</div><div></div><div></div><div>5%</div></div>    |

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147653 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 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | AB    | 220      | Total | C    | N   | O   | S | 0       | 1     |
|     |       |          | 1708  | 1083 | 306 | 312 | 7 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AB    | 7       | ACE      | -      | acetylation | UNP P0A7V0 |
| AB    | 226     | NH2      | -      | amidation   | UNP P0A7V0 |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | AC    | 207      | Total | C    | N   | O   | S | 0       | 1     |
|     |       |          | 1625  | 1028 | 306 | 288 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| AC    | 207     | NH2      | -      | amidation | UNP P0A7V3 |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | AD    | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | AE    | 152      | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 1109  | 689 | 212 | 202 | 6 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AE    | 8       | ACE      | -      | acetylation | UNP P0A7W1 |
| AE    | 159     | NH2      | -      | amidation   | UNP P0A7W1 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | AF    | 101      | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 818   | 515 | 149 | 148 | 6 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| AF    | 101     | NH2      | -      | amidation | UNP P02358 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | AG    | 152      | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 1178  | 732 | 227 | 215 | 4 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AG    | 1       | ACE      | -      | acetylation | UNP P02359 |
| AG    | 152     | NH2      | -      | amidation   | UNP P02359 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | AH    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | AI    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1025  | 636 | 206 | 180 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AI    | 2       | ACE      | -      | acetylation | UNP P0A7X3 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | AJ    | 100      | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 790   | 495 | 151 | 143 | 1 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AJ    | 4       | ACE      | -      | acetylation | UNP P0A7R5 |
| AJ    | 103     | NH2      | -      | amidation   | UNP P0A7R5 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | AK    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 880   | 542 | 174 | 161 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AK    | 11      | ACE      | -      | acetylation | UNP P0A7R9 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | AL    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | AM    | 114      | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 877   | 541 | 178 | 155 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| AM    | 114     | NH2      | -      | amidation | UNP P0A7S9 |

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



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | AN    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | AO    | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | AP    | 81       | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 639   | 400 | 127 | 111 | 1 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| AP    | 81      | NH2      | -      | amidation | UNP P0A7T3 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | AQ    | 82       | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 652   | 413 | 122 | 114 | 3 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AQ    | 2       | ACE      | -      | acetylation | UNP P0AG63 |
| AQ    | 83      | NH2      | -      | amidation   | UNP P0AG63 |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 17  | AR    | 57       | Total | C   | N  | O  | 0       | 1     |
|     |       |          | 459   | 290 | 87 | 82 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AR    | 18      | ACE      | -      | acetylation | UNP P0A7T7 |

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| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| AR    | 74      | NH2      | -      | amidation | UNP P0A7T7 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | AS    | 81       | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 641   | 410 | 121 | 108 | 2 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AS    | 1       | ACE      | -      | acetylation | UNP P0A7U3 |
| AS    | 81      | NH2      | -      | amidation   | UNP P0A7U3 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | AT    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 668   | 413 | 137 | 115 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AT    | 1       | ACE      | -      | acetylation | UNP P0A7U7 |

- Molecule 20 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 20  | AU    | 53       | Total | C   | N  | O  | S | 0       | 1     |
|     |       |          | 429   | 267 | 87 | 74 | 1 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AU    | 2       | ACE      | -      | acetylation | UNP P68679 |
| AU    | 54      | NH2      | -      | amidation   | UNP P68679 |

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 21  | AA    | 1530     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32828 | 14642 | 6024 | 10633 | 1529 |         |       |

- Molecule 22 is a RNA chain called fMet-Val-tRNA-Val.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 22  | A1    | 76       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1627  | 728 | 292 | 531 | 75 | 1 |         |       |

- Molecule 23 is a RNA chain called 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 23  | A2    | 15       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 309   | 140 | 46 | 109 | 14 |         |       |

- Molecule 24 is a RNA chain called tRNA-fMet.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 24  | A3    | 77       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1642  | 734 | 297 | 534 | 76 | 1 |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 25  | BC    | 272      | Total | C    | N   | O   | S | 0       | 1     |
|     |       |          | 2083  | 1288 | 424 | 364 | 7 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| BC    | 272     | NH2      | -      | amidation | UNP P60422 |

- Molecule 26 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | BD    | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | BE    | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | BF    | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1420  | 905 | 251 | 258 | 6 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | BG    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | BH    | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | BI    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | BJ    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | BK    | 123      | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 939   | 587 | 181 | 165 | 6 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| BK    | 123     | NH2      | -      | amidation | UNP P0ADY3 |

- Molecule 34 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | BL    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | BM    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | BN    | 121      | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 961   | 593 | 197 | 166 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| BN    | 121     | NH2      | -      | amidation | UNP P0AG44 |

- Molecule 37 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 37  | BO    | 116      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |  |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | BP    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 39  | BQ    | 117      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |  |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | BR    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | BS    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | BT    | 94       | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 739   | 466 | 140 | 131 | 2 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| BT    | 94      | NH2      | -      | amidation | UNP P0ADZ0 |

- Molecule 43 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 43  | BU    | 103      | Total | C   | N   | O   | 0       | 1     |
|     |       |          | 780   | 492 | 147 | 141 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| BU    | 103     | NH2      | -      | amidation | UNP P60624 |

- Molecule 44 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | BV    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | BW    | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 599   | 369 | 120 | 109 | 1 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| BW    | 5       | ACE      | -      | acetylation | UNP P0A7L8 |

- Molecule 46 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | BX    | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| BX    | -1      | ACE      | -      | acetylation | UNP P0A7M2 |

- Molecule 47 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 47  | BY    | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 48  | BZ    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49  | B0    | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 50  | B1    | 52       | Total | C   | N  | O  | 0       | 1     |
|     |       |          | 413   | 265 | 76 | 72 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| B1    | 2       | ACE      | -      | acetylation | UNP P0A7N9 |
| B1    | 53      | NH2      | -      | amidation   | UNP P0A7N9 |

- Molecule 51 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 51  | B2    | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 52  | B3    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 53  | B4    | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 54  | BA    | 2903     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62317 | 27801 | 11467 | 20147 | 2902 |         |       |

- Molecule 55 is a RNA chain called 5S ribosomal RNA.

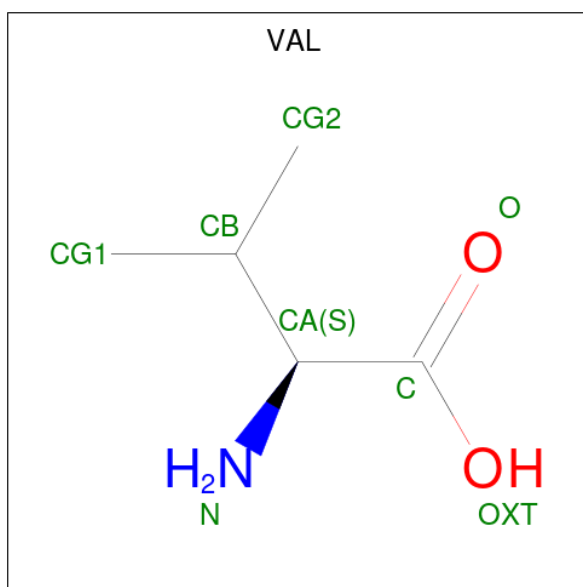
| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 55  | BB    | 117      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2504  | 1116 | 459 | 813 | 116 |         |       |

- Molecule 56 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56  | B5    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1658  | 1038 | 302 | 312 | 6 |         |       |

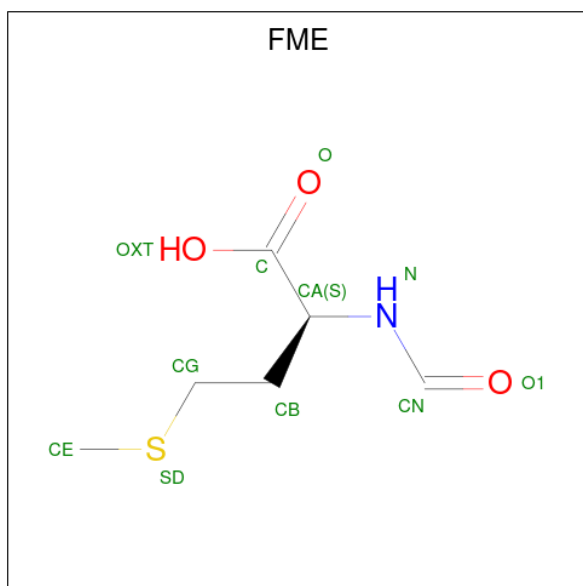
- Molecule 57 is VALINE (CCD ID: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).





| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 57  | A1    | 1        | Total | C | N | O | 0       |
|     |       |          | 7     | 5 | 1 | 1 |         |

- Molecule 58 is N-FORMYLMETHIONINE (CCD ID: FME) (formula:  $C_6H_{11}NO_3S$ ).

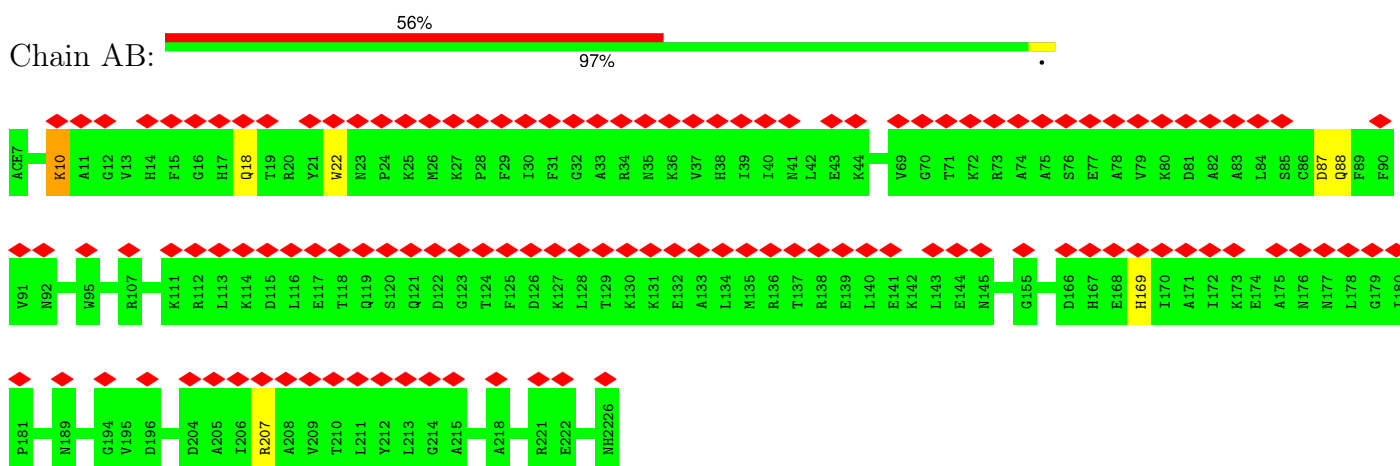


| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 58  | A1    | 1        | Total | C | N | O | S | 0       |
|     |       |          | 10    | 6 | 1 | 2 | 1 |         |

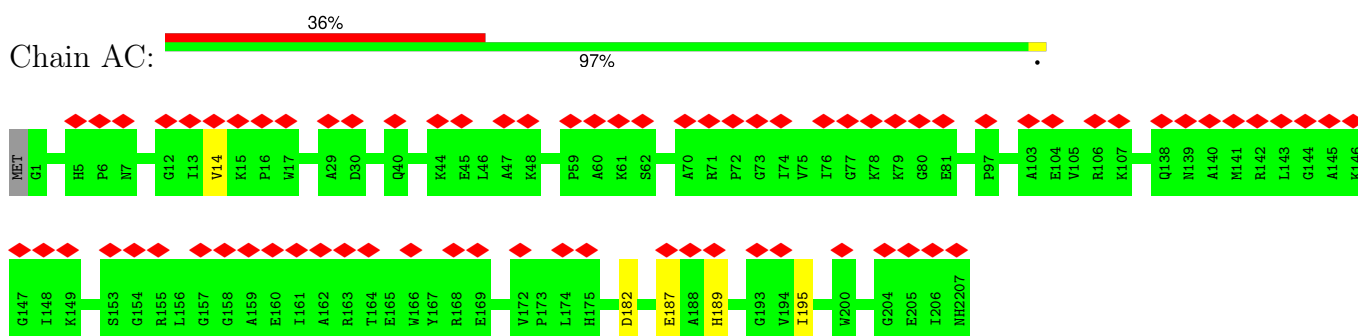
### 3 Residue-property plots

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

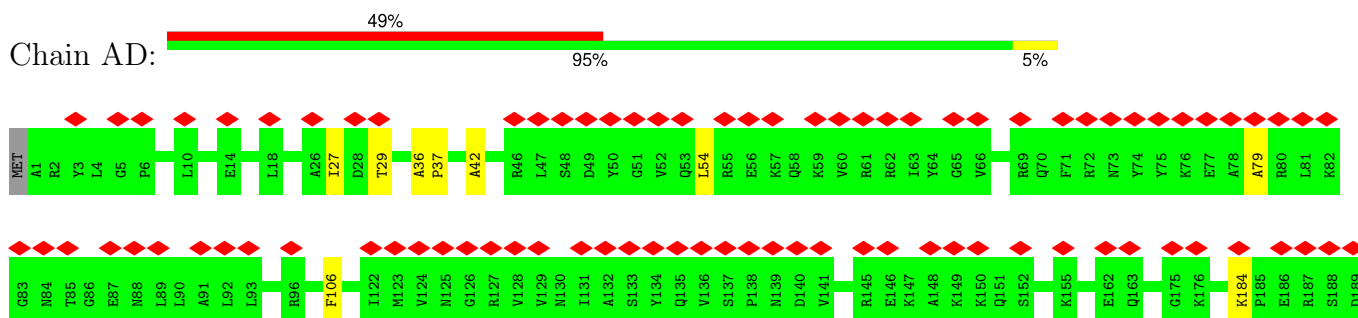
#### • Molecule 1: 30S ribosomal protein S2

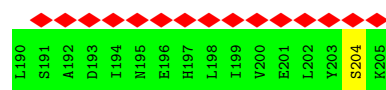


#### • Molecule 2: 30S ribosomal protein S3

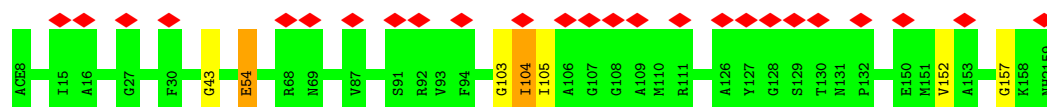


#### • Molecule 3: 30S ribosomal protein S4

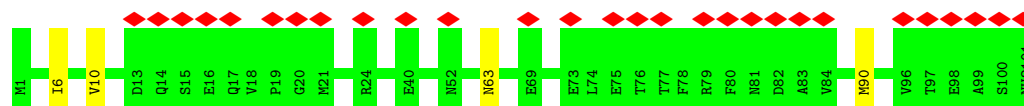




- Molecule 4: 30S ribosomal protein S5



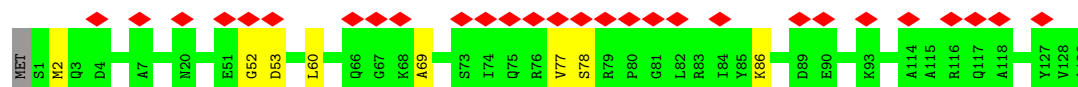
- Molecule 5: 30S ribosomal protein S6



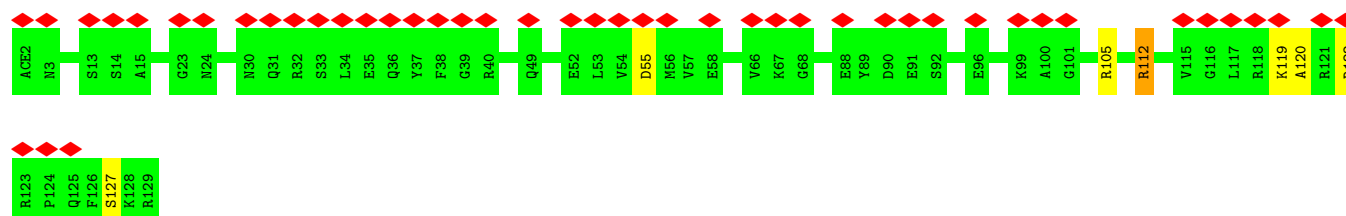
- Molecule 6: 30S ribosomal protein S7



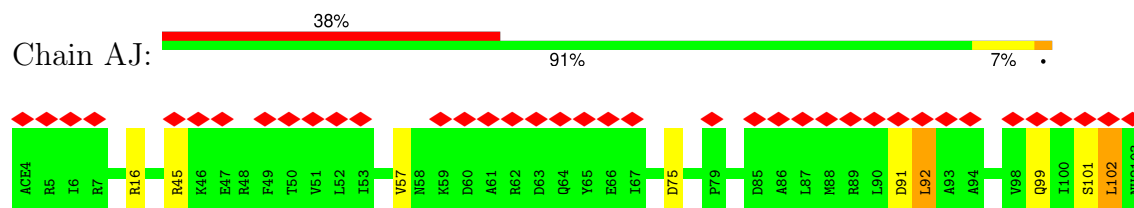
- Molecule 7: 30S ribosomal protein S8



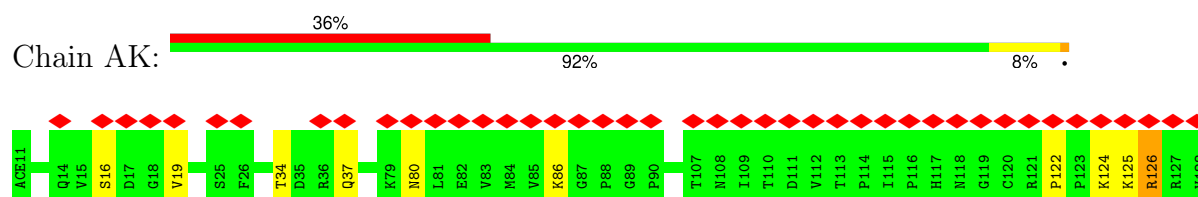
- Molecule 8: 30S ribosomal protein S9



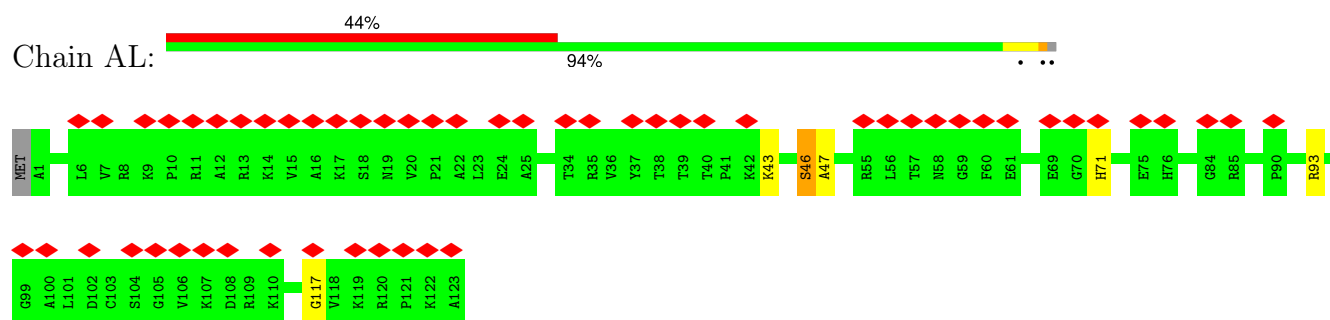
- Molecule 9: 30S ribosomal protein S10



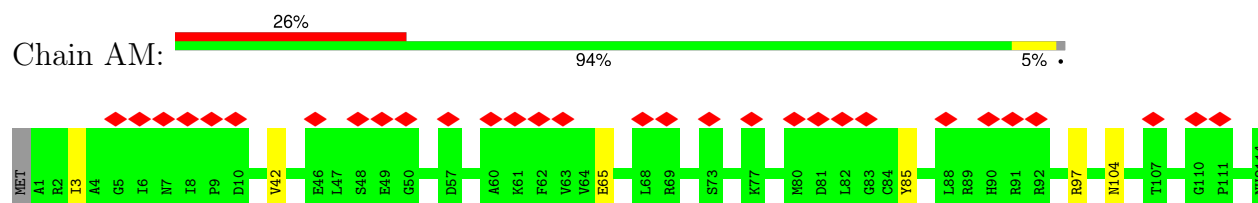
- Molecule 10: 30S ribosomal protein S11



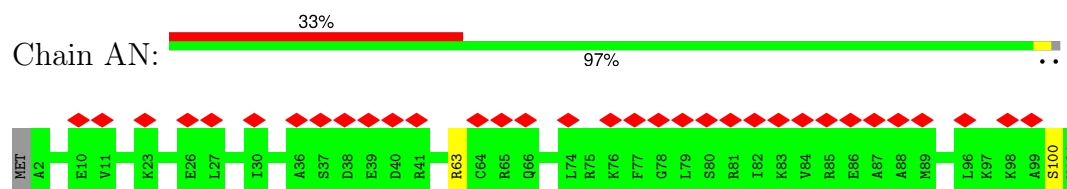
- Molecule 11: 30S ribosomal protein S12



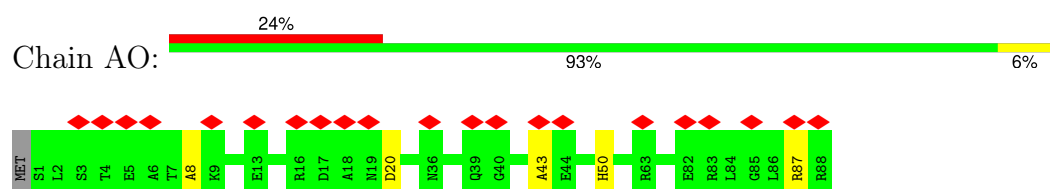
- Molecule 12: 30S ribosomal protein S13



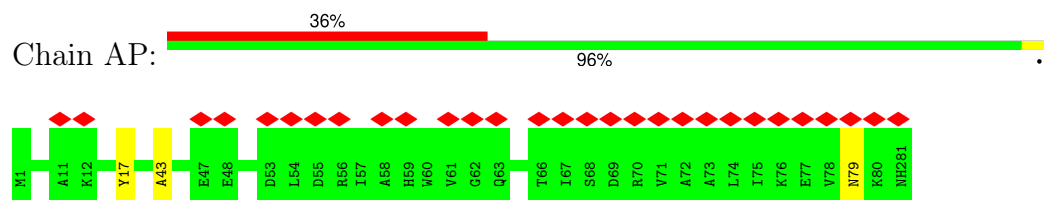
- Molecule 13: 30S ribosomal protein S14



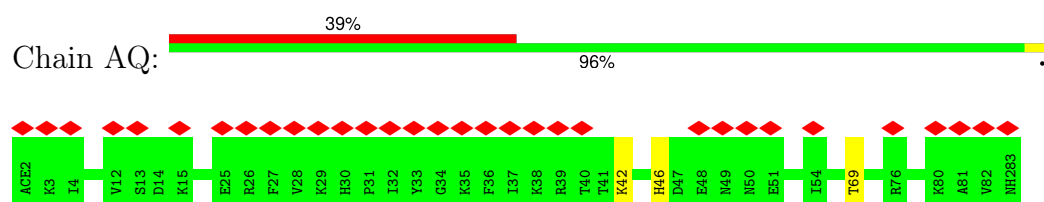
- Molecule 14: 30S ribosomal protein S15



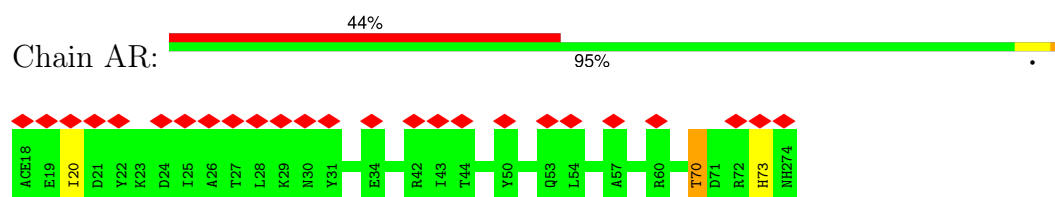
- Molecule 15: 30S ribosomal protein S16



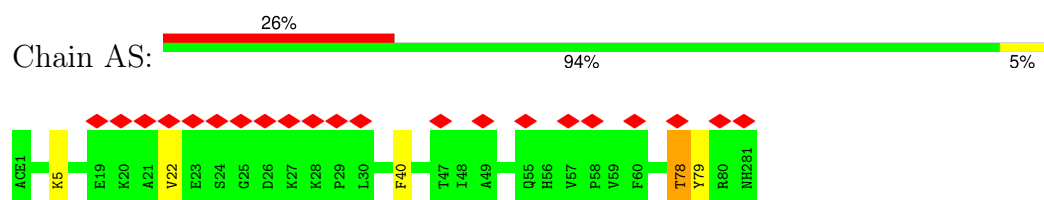
- Molecule 16: 30S ribosomal protein S17



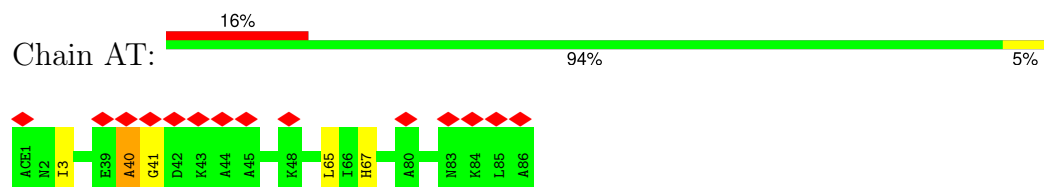
- Molecule 17: 30S ribosomal protein S18



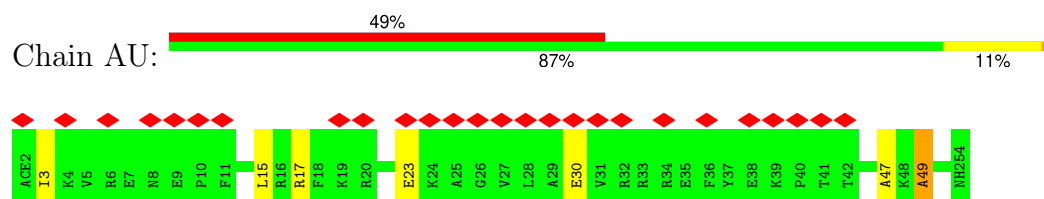
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



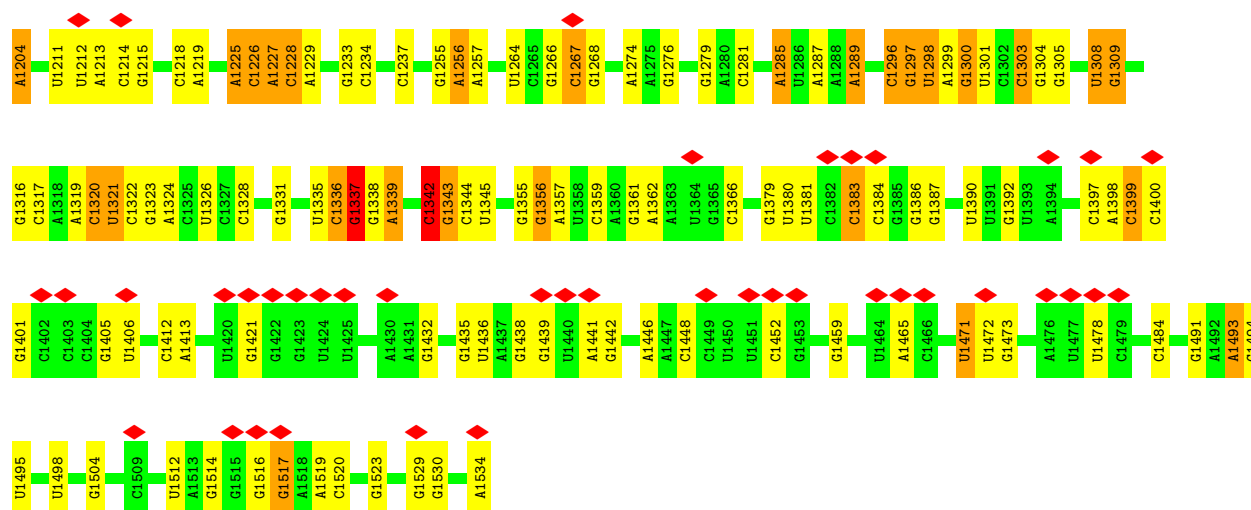
- Molecule 20: 30S ribosomal protein S21



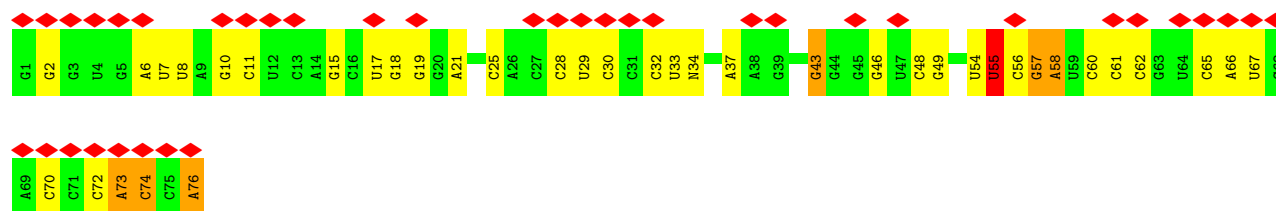
- Molecule 21: 16S ribosomal RNA







• Molecule 22: fMet-Val-tRNA-Val



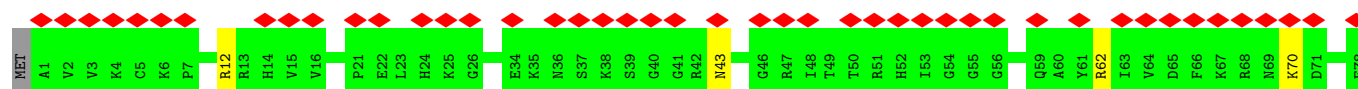
• Molecule 23: 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'

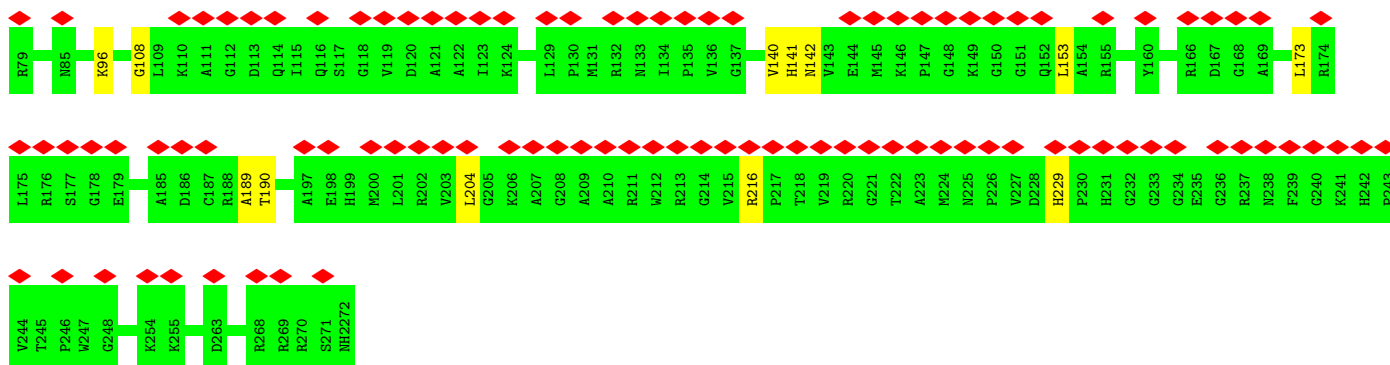


• Molecule 24: tRNA-fMet

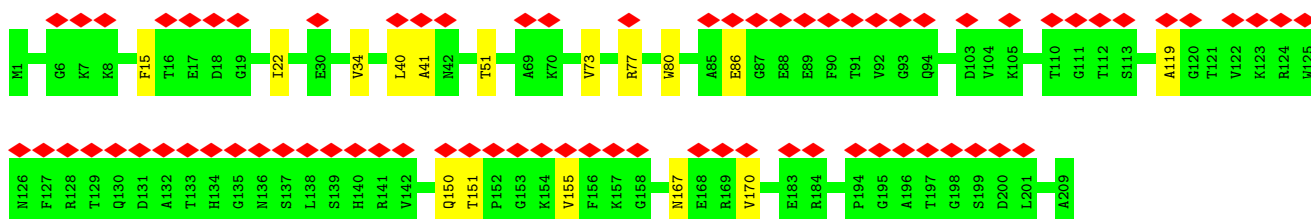


• Molecule 25: 50S ribosomal protein L2

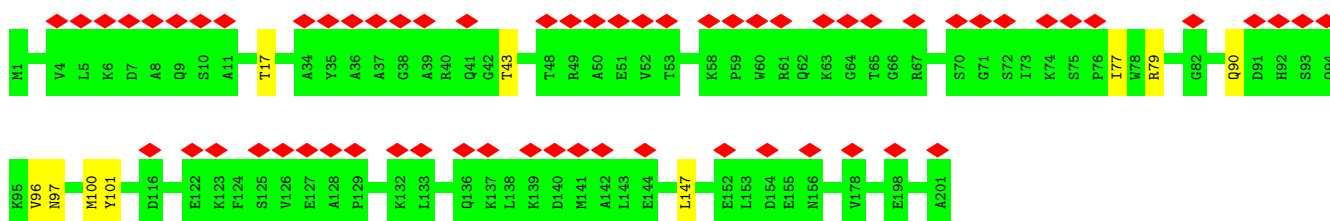




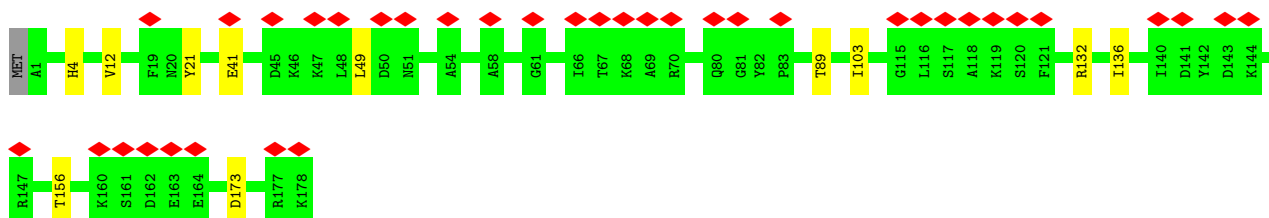
• Molecule 26: 50S ribosomal protein L3



• Molecule 27: 50S ribosomal protein L4



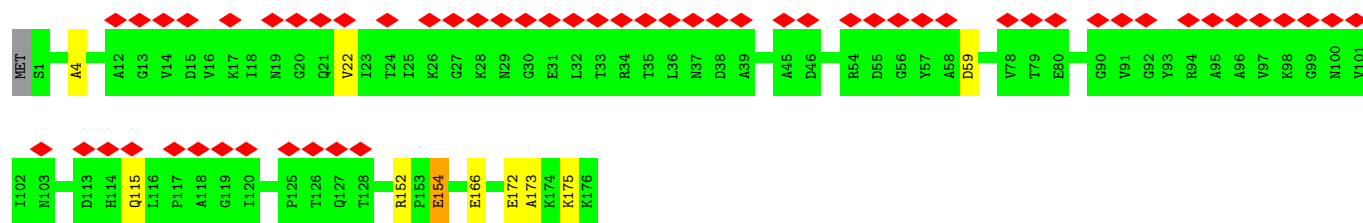
• Molecule 28: 50S ribosomal protein L5



• Molecule 29: 50S ribosomal protein L6

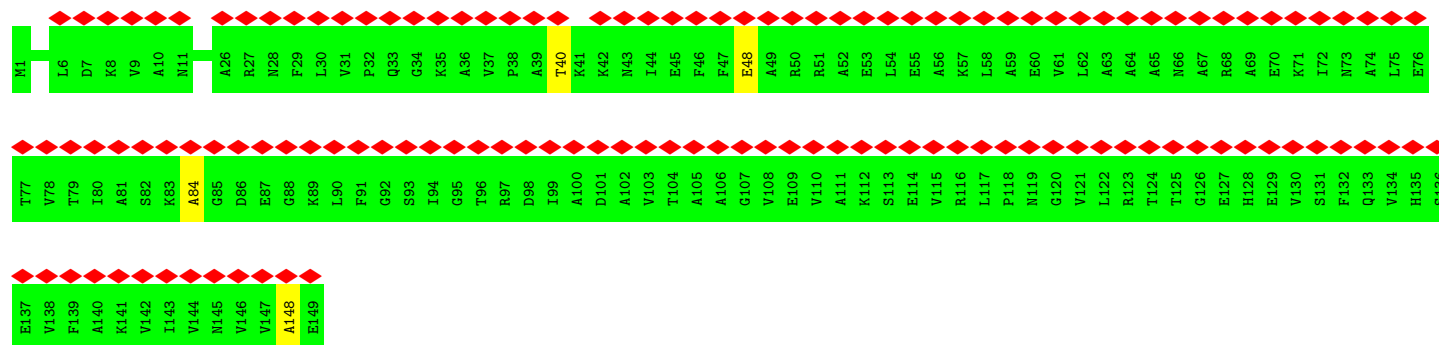






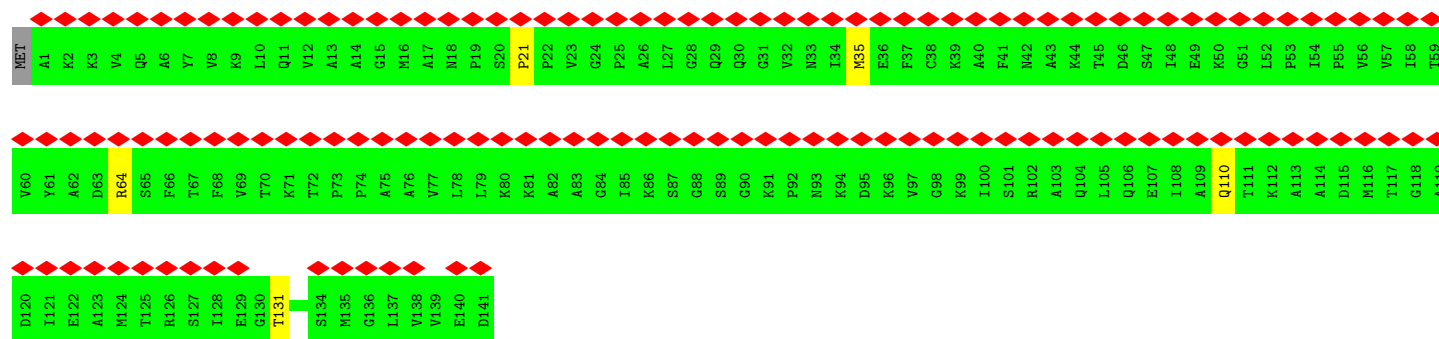
- Molecule 30: 50S ribosomal protein L9

Chain BH: 87%  
97%



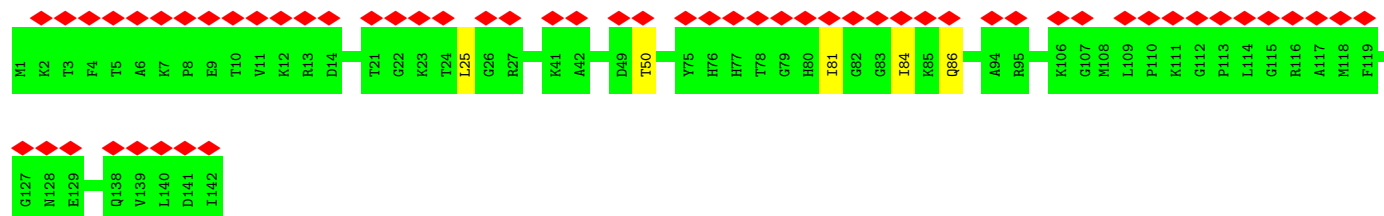
- Molecule 31: 50S ribosomal protein L11

Chain BI: 96%  
96%

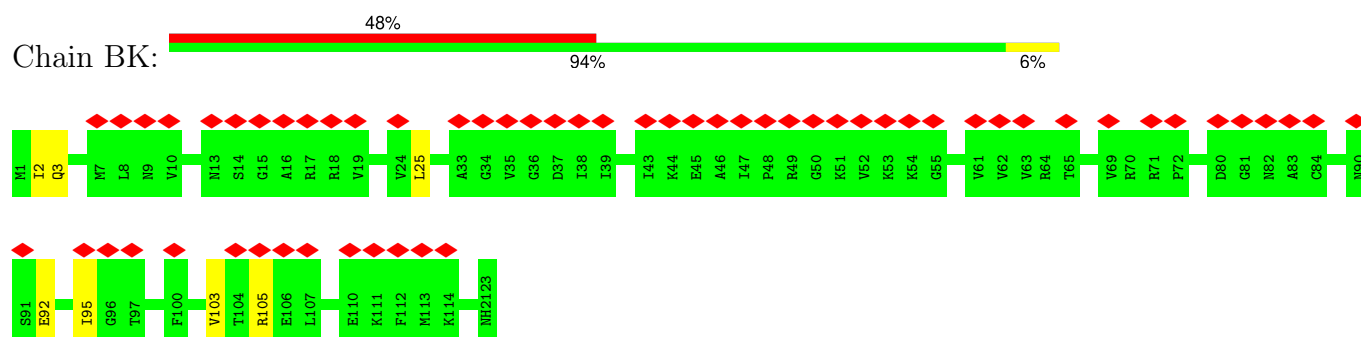


- Molecule 32: 50S ribosomal protein L13

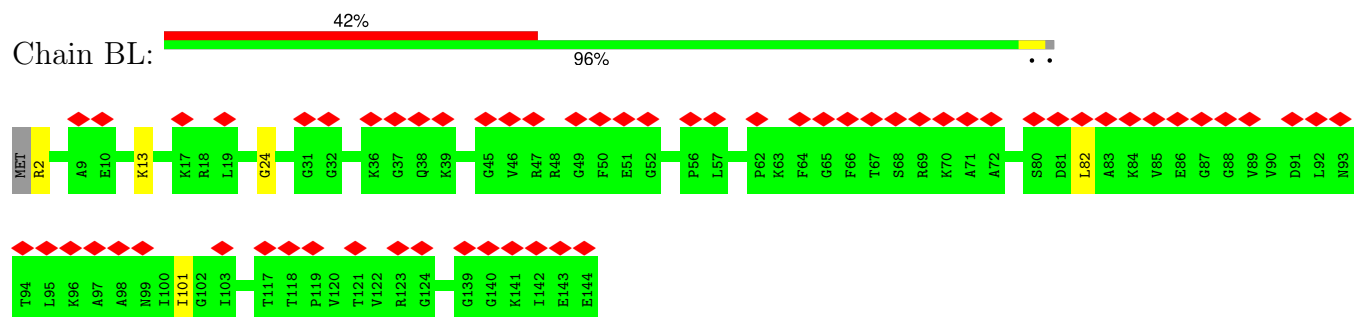
Chain BJ: 41%  
96%



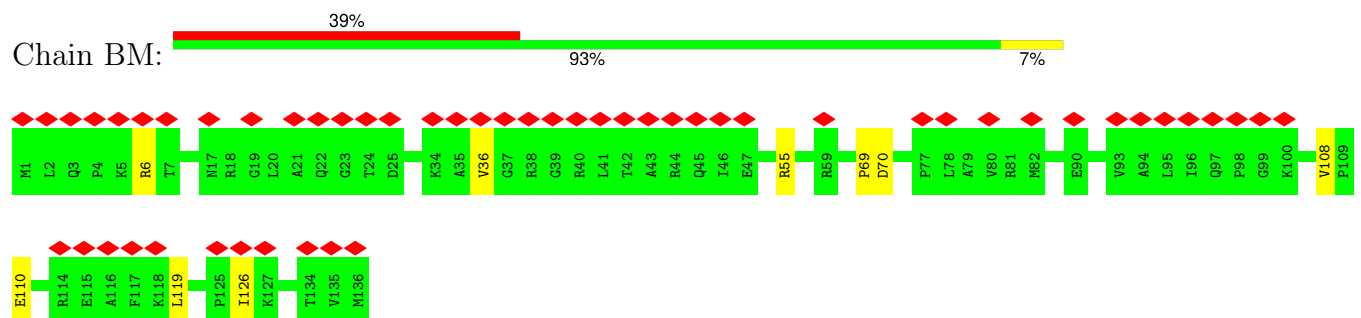
- Molecule 33: 50S ribosomal protein L14



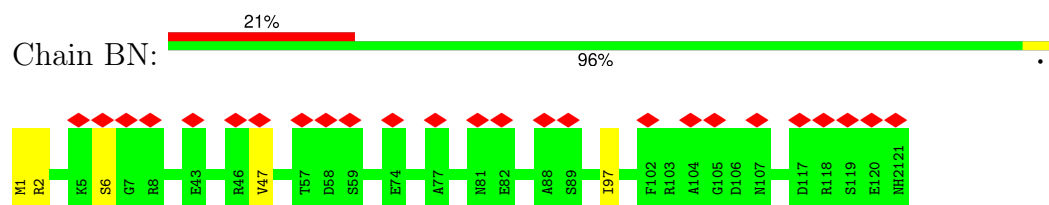
- Molecule 34: 50S ribosomal protein L15



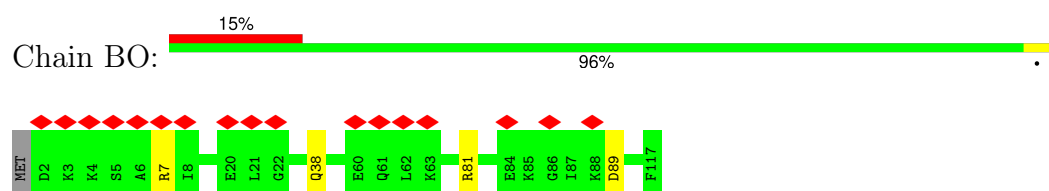
- Molecule 35: 50S ribosomal protein L16



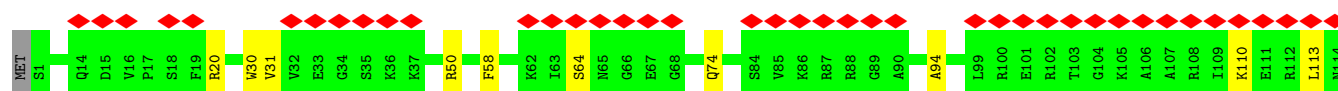
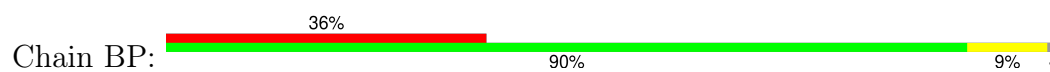
- Molecule 36: 50S ribosomal protein L17



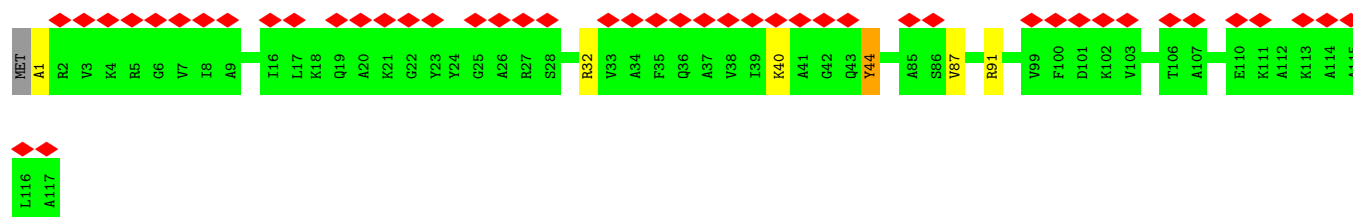
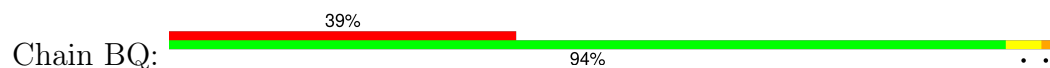
- Molecule 37: 50S ribosomal protein L18



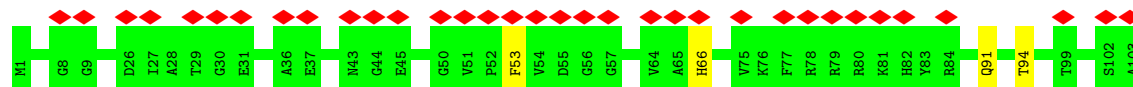
- Molecule 38: 50S ribosomal protein L19



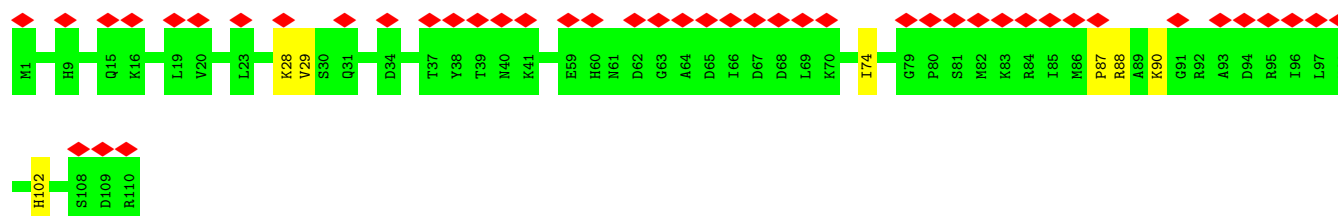
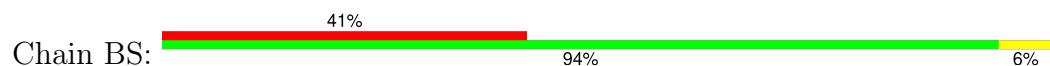
- Molecule 39: 50S ribosomal protein L20



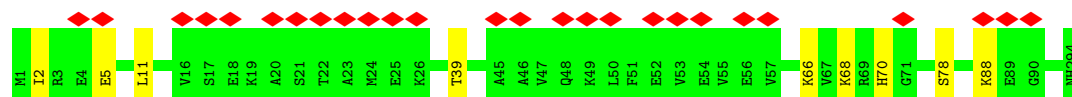
- Molecule 40: 50S ribosomal protein L21



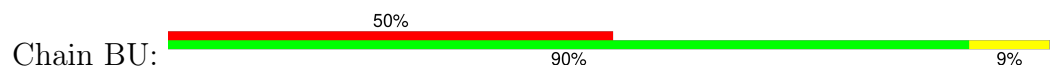
- Molecule 41: 50S ribosomal protein L22

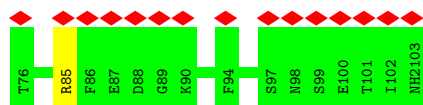


- Molecule 42: 50S ribosomal protein L23

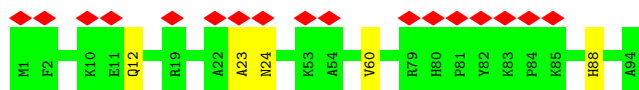


- Molecule 43: 50S ribosomal protein L24

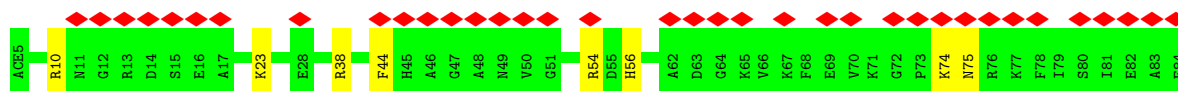




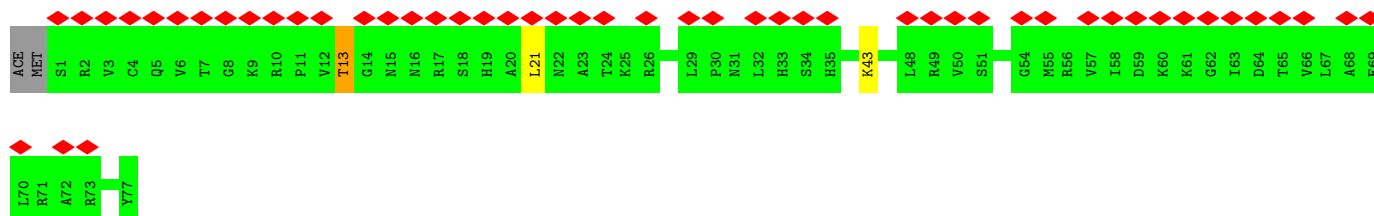
- Molecule 44: 50S ribosomal protein L25



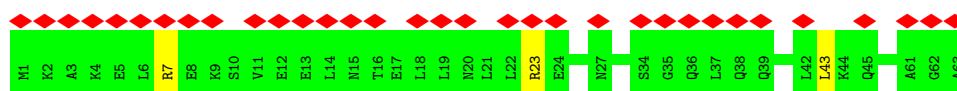
- Molecule 45: 50S ribosomal protein L27



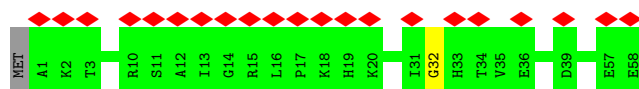
- Molecule 46: 50S ribosomal protein L28



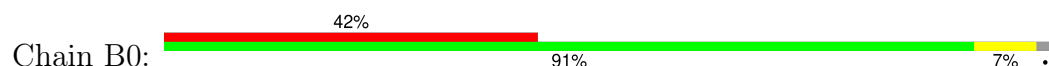
- Molecule 47: 50S ribosomal protein L29

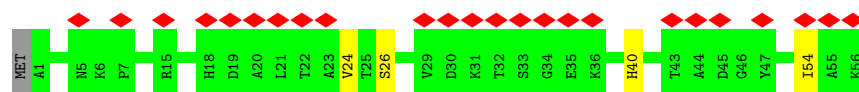


- Molecule 48: 50S ribosomal protein L30

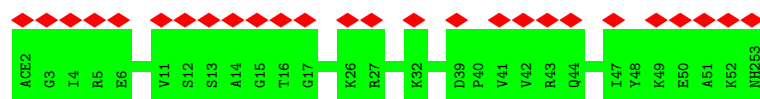


- Molecule 49: 50S ribosomal protein L32

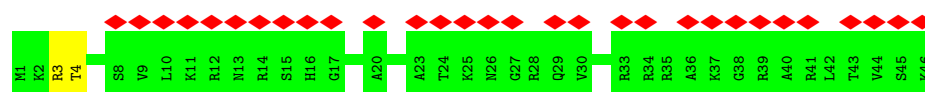




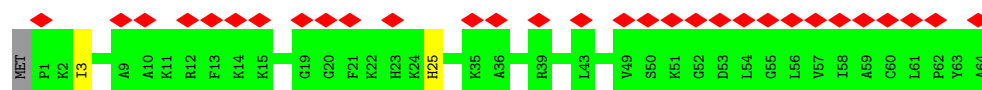
- Molecule 50: 50S ribosomal protein L33



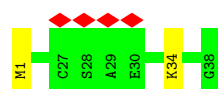
- Molecule 51: 50S ribosomal protein L34



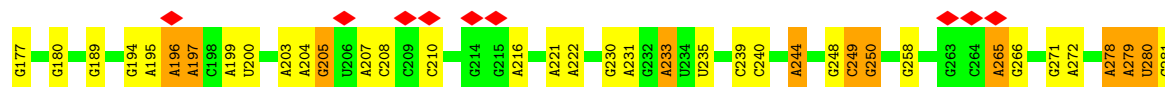
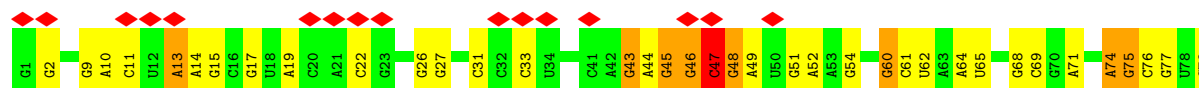
- Molecule 52: 50S ribosomal protein L35



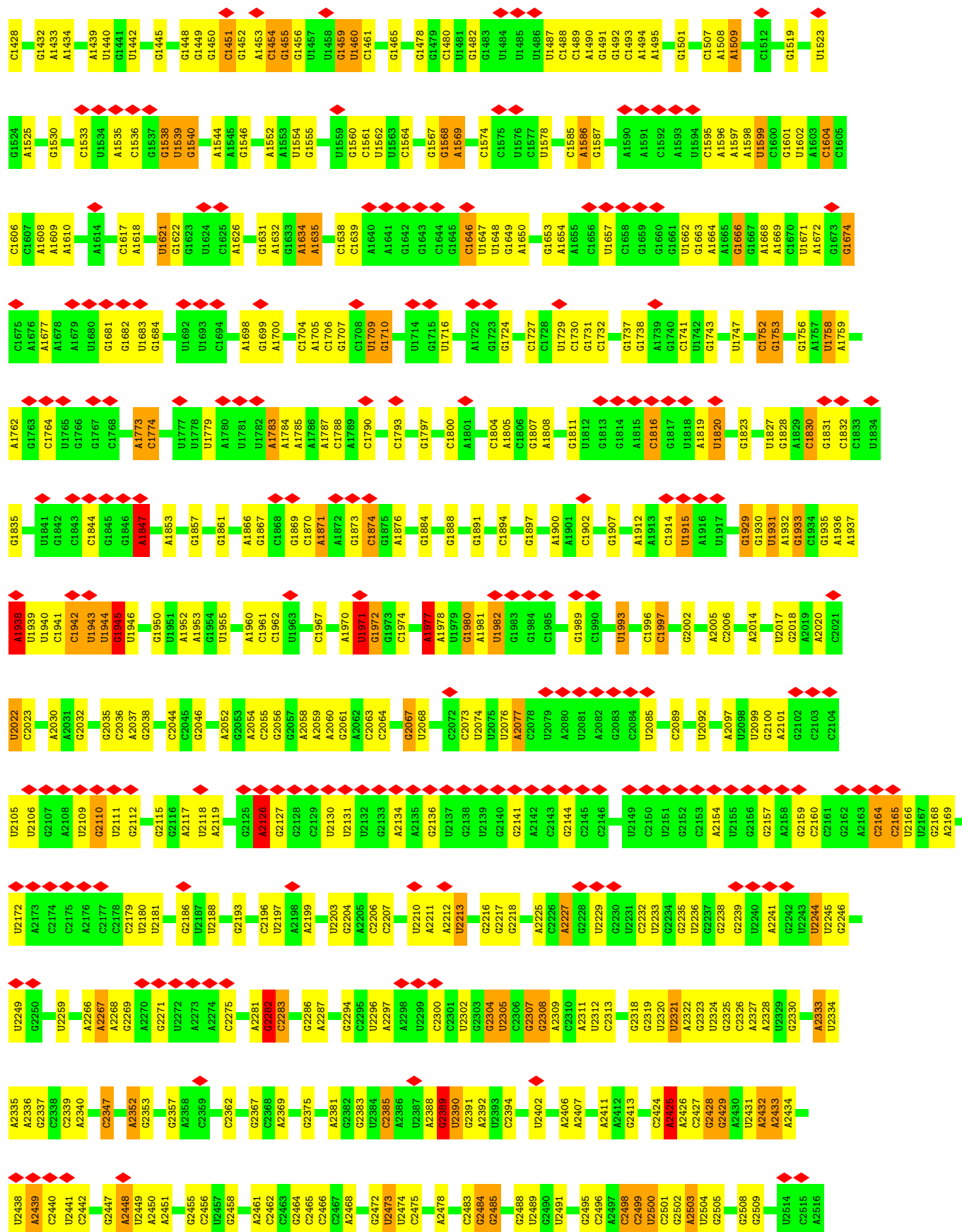
- Molecule 53: 50S ribosomal protein L36

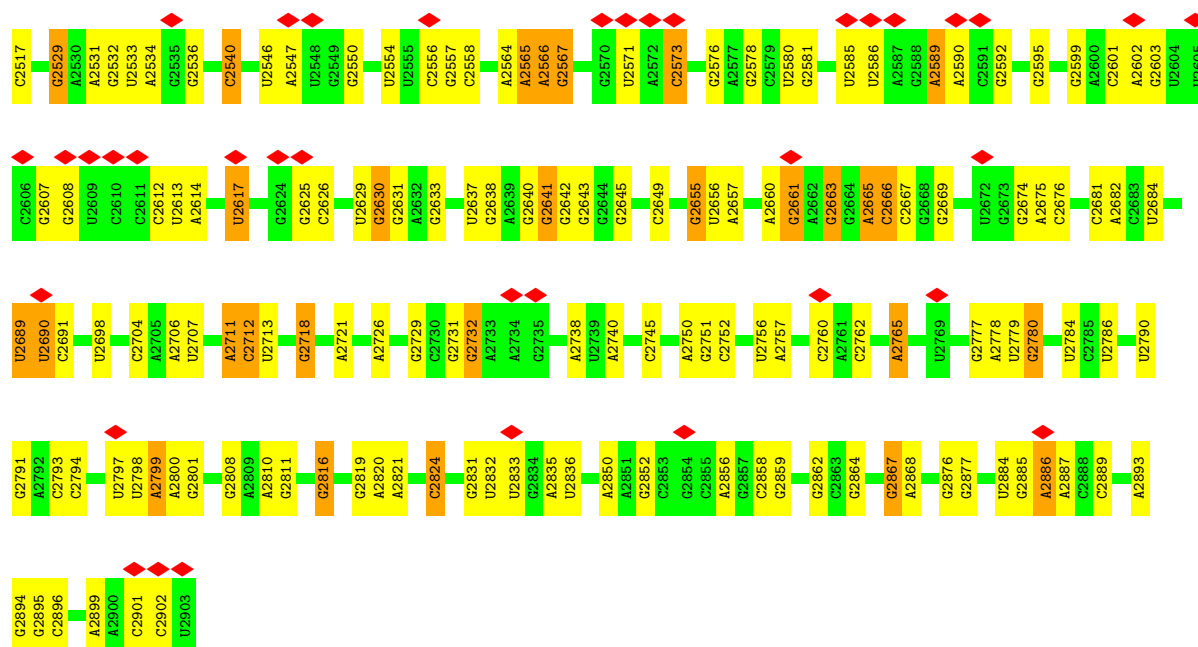


- Molecule 54: 23S ribosomal RNA

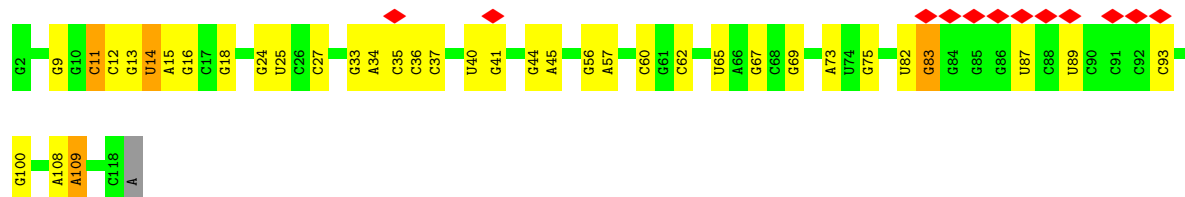




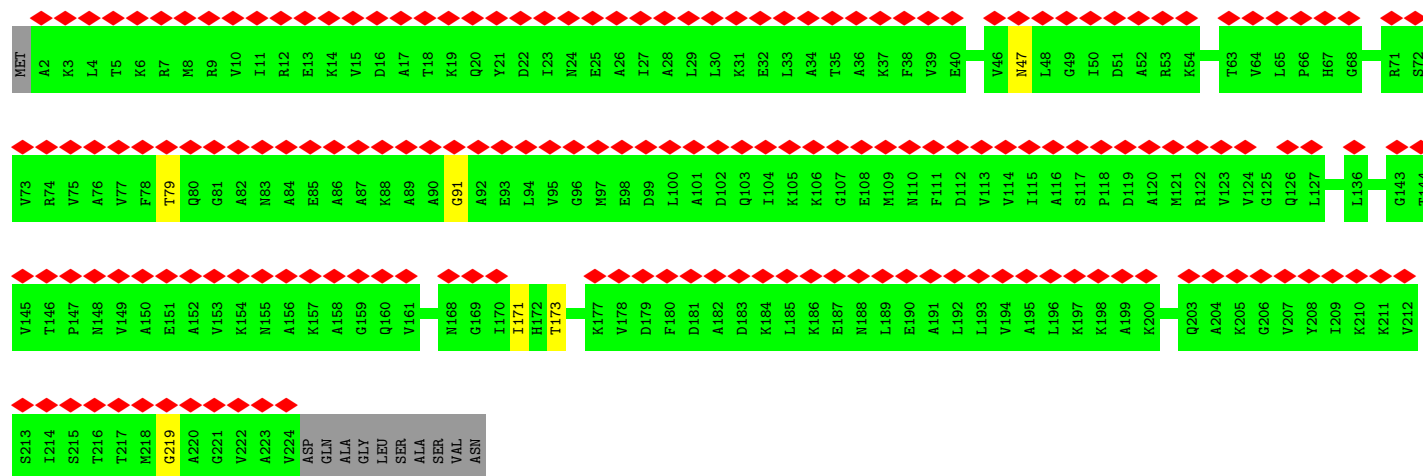
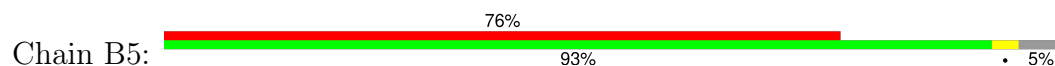




• Molecule 55: 5S ribosomal RNA



• Molecule 56: 50S ribosomal protein L1





## 4 Experimental information

| Property                             | Value                   | Source    |
|--------------------------------------|-------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE         | Depositor |
| Imposed symmetry                     | POINT, C1               | Depositor |
| Number of particles used             | 1904                    | Depositor |
| Resolution determination method      | FSC 0.5 CUT-OFF         | Depositor |
| CTF correction method                | local                   | Depositor |
| Microscope                           | FEI/PHILIPS CM200FEG    | Depositor |
| Voltage (kV)                         | 160                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 20                      | Depositor |
| Minimum defocus (nm)                 | 500                     | Depositor |
| Maximum defocus (nm)                 | 2000                    | Depositor |
| Magnification                        | 162740                  | Depositor |
| Image detector                       | GENERIC TVIPS (4k x 4k) | Depositor |
| Maximum map value                    | 157.537                 | Depositor |
| Minimum map value                    | -94.382                 | Depositor |
| Average map value                    | -1.909                  | Depositor |
| Map value standard deviation         | 16.235                  | Depositor |
| Recommended contour level            | 22                      | Depositor |
| Map size ( $\text{\AA}$ )            | 358.4, 358.4, 358.4     | wwPDB     |
| Map dimensions                       | 128, 128, 128           | wwPDB     |
| Map angles ( $^\circ$ )              | 90, 90, 90              | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 2.8, 2.8, 2.8           | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, H2U, FME, 4SU, OMC, PSU, CM0, 6MZ, 7MG, NH2, ACE

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   | AB    | 0.94         | 0/1736      | 1.39        | 4/2340 (0.2%)   |
| 2   | AC    | 0.94         | 0/1651      | 1.36        | 0/2225          |
| 3   | AD    | 0.95         | 0/1665      | 1.44        | 12/2227 (0.5%)  |
| 4   | AE    | 0.95         | 0/1119      | 1.48        | 8/1506 (0.5%)   |
| 5   | AF    | 0.96         | 0/835       | 1.43        | 0/1128          |
| 6   | AG    | 0.95         | 0/1188      | 1.42        | 7/1593 (0.4%)   |
| 7   | AH    | 0.89         | 0/989       | 1.35        | 2/1326 (0.2%)   |
| 8   | AI    | 0.99         | 0/1035      | 1.46        | 5/1377 (0.4%)   |
| 9   | AJ    | 0.97         | 0/797       | 1.41        | 6/1079 (0.6%)   |
| 10  | AK    | 0.97         | 0/894       | 1.42        | 5/1207 (0.4%)   |
| 11  | AL    | 0.97         | 0/969       | 1.37        | 3/1300 (0.2%)   |
| 12  | AM    | 0.99         | 0/884       | 1.43        | 1/1181 (0.1%)   |
| 13  | AN    | 0.98         | 0/817       | 1.36        | 2/1088 (0.2%)   |
| 14  | AO    | 0.93         | 0/722       | 1.45        | 3/964 (0.3%)    |
| 15  | AP    | 0.94         | 0/648       | 1.44        | 2/870 (0.2%)    |
| 16  | AQ    | 0.92         | 0/658       | 1.38        | 0/883           |
| 17  | AR    | 0.97         | 0/463       | 1.41        | 3/623 (0.5%)    |
| 18  | AS    | 0.99         | 0/653       | 1.50        | 7/879 (0.8%)    |
| 19  | AT    | 0.91         | 0/672       | 1.48        | 3/890 (0.3%)    |
| 20  | AU    | 1.00         | 0/431       | 1.74        | 9/572 (1.6%)    |
| 21  | AA    | 0.99         | 0/36759     | 1.15        | 66/57346 (0.1%) |
| 22  | A1    | 1.00         | 0/1668      | 1.14        | 3/2595 (0.1%)   |
| 23  | A2    | 1.07         | 0/343       | 1.30        | 3/531 (0.6%)    |
| 24  | A3    | 0.99         | 0/1722      | 1.19        | 7/2685 (0.3%)   |
| 25  | BC    | 0.94         | 0/2121      | 1.49        | 6/2852 (0.2%)   |
| 26  | BD    | 0.88         | 0/1586      | 1.51        | 0/2134          |
| 27  | BE    | 0.86         | 0/1571      | 1.45        | 4/2113 (0.2%)   |
| 28  | BF    | 0.89         | 0/1444      | 1.42        | 0/1937          |
| 29  | BG    | 0.89         | 0/1343      | 1.47        | 9/1816 (0.5%)   |
| 30  | BH    | 0.86         | 0/1122      | 1.43        | 4/1515 (0.3%)   |
| 31  | BI    | 0.86         | 0/1046      | 1.46        | 2/1410 (0.1%)   |
| 32  | BJ    | 0.93         | 0/1152      | 1.49        | 3/1551 (0.2%)   |

| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 33  | BK    | 0.93         | 0/947    | 1.48        | 3/1268 (0.2%)     |
| 34  | BL    | 0.92         | 0/1054   | 1.49        | 2/1403 (0.1%)     |
| 35  | BM    | 0.91         | 0/1093   | 1.46        | 1/1460 (0.1%)     |
| 36  | BN    | 0.94         | 0/973    | 1.50        | 2/1301 (0.2%)     |
| 37  | BO    | 0.89         | 0/902    | 1.45        | 2/1209 (0.2%)     |
| 38  | BP    | 0.92         | 0/929    | 1.52        | 4/1242 (0.3%)     |
| 39  | BQ    | 0.90         | 0/960    | 1.42        | 2/1278 (0.2%)     |
| 40  | BR    | 0.88         | 0/829    | 1.43        | 1/1107 (0.1%)     |
| 41  | BS    | 0.91         | 0/864    | 1.50        | 5/1156 (0.4%)     |
| 42  | BT    | 0.84         | 0/744    | 1.54        | 4/994 (0.4%)      |
| 43  | BU    | 0.88         | 0/787    | 1.45        | 2/1051 (0.2%)     |
| 44  | BV    | 0.88         | 0/766    | 1.44        | 1/1025 (0.1%)     |
| 45  | BW    | 0.94         | 0/604    | 1.65        | 2/799 (0.3%)      |
| 46  | BX    | 0.90         | 0/635    | 1.54        | 2/848 (0.2%)      |
| 47  | BY    | 0.90         | 0/510    | 1.46        | 0/677             |
| 48  | BZ    | 0.90         | 0/453    | 1.50        | 0/605             |
| 49  | B0    | 0.99         | 0/450    | 1.54        | 2/599 (0.3%)      |
| 50  | B1    | 0.88         | 0/417    | 1.35        | 0/556             |
| 51  | B2    | 0.97         | 0/380    | 1.55        | 0/498             |
| 52  | B3    | 0.95         | 0/513    | 1.44        | 1/676 (0.1%)      |
| 53  | B4    | 0.89         | 0/303    | 1.49        | 0/397             |
| 54  | BA    | 0.83         | 0/69796  | 1.14        | 122/108888 (0.1%) |
| 55  | BB    | 0.84         | 0/2800   | 1.10        | 1/4367 (0.0%)     |
| 56  | B5    | 0.84         | 0/1673   | 1.43        | 3/2255 (0.1%)     |
| All | All   | 0.90         | 0/160085 | 1.23        | 351/239402 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | AD    | 0                   | 1                   |
| 8   | AI    | 0                   | 1                   |
| 14  | AO    | 0                   | 1                   |
| 21  | AA    | 0                   | 372                 |
| 22  | A1    | 0                   | 21                  |
| 23  | A2    | 0                   | 5                   |
| 24  | A3    | 0                   | 7                   |
| 27  | BE    | 0                   | 1                   |
| 37  | BO    | 0                   | 1                   |
| 39  | BQ    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 45  | BW    | 0                   | 1                   |
| 54  | BA    | 0                   | 726                 |
| 55  | BB    | 0                   | 20                  |
| All | All   | 0                   | 1158                |

There are no bond length outliers.

All (351) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AB    | 10   | LYS  | CA-C-N      | 8.89  | 137.70      | 121.70   |
| 1   | AB    | 10   | LYS  | C-N-CA      | 8.89  | 137.70      | 121.70   |
| 45  | BW    | 74   | LYS  | CA-C-N      | 8.81  | 137.56      | 121.70   |
| 45  | BW    | 74   | LYS  | C-N-CA      | 8.81  | 137.56      | 121.70   |
| 20  | AU    | 30   | GLU  | CA-C-N      | 8.68  | 137.33      | 121.70   |
| 20  | AU    | 30   | GLU  | C-N-CA      | 8.68  | 137.33      | 121.70   |
| 6   | AG    | 4    | ARG  | CA-C-N      | 8.68  | 137.31      | 121.70   |
| 6   | AG    | 4    | ARG  | C-N-CA      | 8.68  | 137.31      | 121.70   |
| 54  | BA    | 1451 | C    | C2'-C3'-O3' | 8.60  | 122.40      | 109.50   |
| 24  | A3    | 72   | C    | O3'-P-O5'   | 8.45  | 116.67      | 104.00   |
| 18  | AS    | 78   | THR  | CA-C-N      | 8.30  | 136.65      | 121.70   |
| 18  | AS    | 78   | THR  | C-N-CA      | 8.30  | 136.65      | 121.70   |
| 46  | BX    | 13   | THR  | CA-C-N      | 7.96  | 128.29      | 122.16   |
| 46  | BX    | 13   | THR  | C-N-CA      | 7.96  | 128.29      | 122.16   |
| 54  | BA    | 1378 | A    | C1'-O4'-C4' | -7.85 | 102.05      | 109.90   |
| 54  | BA    | 1132 | U    | C4'-C3'-O3' | 7.74  | 121.01      | 109.40   |
| 21  | AA    | 365  | U    | C1'-O4'-C4' | -7.61 | 102.29      | 109.90   |
| 21  | AA    | 465  | A    | C1'-O4'-C4' | -7.49 | 102.21      | 109.70   |
| 21  | AA    | 1060 | U    | P-O3'-C3'   | 7.31  | 131.17      | 120.20   |
| 4   | AE    | 54   | GLU  | CA-C-N      | 7.25  | 124.81      | 120.24   |
| 4   | AE    | 54   | GLU  | C-N-CA      | 7.25  | 124.81      | 120.24   |
| 23  | A2    | 92   | U    | C5'-C4'-C3' | -7.25 | 105.13      | 116.00   |
| 22  | A1    | 76   | A    | O4'-C1'-C2' | -7.20 | 98.60       | 105.80   |
| 18  | AS    | 22   | VAL  | CA-C-N      | 7.17  | 134.61      | 121.70   |
| 18  | AS    | 22   | VAL  | C-N-CA      | 7.17  | 134.61      | 121.70   |
| 54  | BA    | 2546 | U    | O3'-P-O5'   | -7.14 | 93.28       | 104.00   |
| 54  | BA    | 961  | C    | C4'-C3'-O3' | 6.87  | 119.71      | 109.40   |
| 41  | BS    | 87   | PRO  | CA-C-N      | 6.87  | 134.06      | 121.70   |
| 41  | BS    | 87   | PRO  | C-N-CA      | 6.87  | 134.06      | 121.70   |
| 54  | BA    | 249  | C    | C2'-C3'-O3' | 6.84  | 119.76      | 109.50   |
| 12  | AM    | 97   | ARG  | NE-CZ-NH2   | 6.80  | 125.32      | 119.20   |
| 8   | AI    | 122  | ARG  | NE-CZ-NH2   | 6.78  | 125.30      | 119.20   |
| 20  | AU    | 15   | LEU  | CA-C-N      | 6.71  | 133.79      | 121.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 20  | AU    | 15   | LEU  | C-N-CA      | 6.71  | 133.79      | 121.70   |
| 10  | AK    | 126  | ARG  | NE-CZ-NH2   | 6.67  | 125.20      | 119.20   |
| 54  | BA    | 1063 | G    | C1'-O4'-C4' | -6.67 | 103.23      | 109.90   |
| 54  | BA    | 989  | G    | O4'-C4'-C3' | 6.60  | 110.60      | 104.00   |
| 24  | A3    | 21   | H2U  | O3'-P-O5'   | -6.59 | 94.11       | 104.00   |
| 1   | AB    | 207  | ARG  | NE-CZ-NH2   | 6.56  | 125.11      | 119.20   |
| 21  | AA    | 1342 | C    | P-O3'-C3'   | 6.54  | 130.01      | 120.20   |
| 54  | BA    | 278  | A    | N9-C1'-C2'  | 6.52  | 121.78      | 112.00   |
| 54  | BA    | 2501 | C    | O4'-C1'-C2' | -6.52 | 99.28       | 105.80   |
| 54  | BA    | 233  | A    | O4'-C1'-C2' | -6.47 | 101.12      | 107.60   |
| 54  | BA    | 1793 | C    | C4'-C3'-C2' | -6.44 | 96.16       | 102.60   |
| 29  | BG    | 175  | LYS  | CA-C-N      | 6.42  | 133.25      | 121.70   |
| 29  | BG    | 175  | LYS  | C-N-CA      | 6.42  | 133.25      | 121.70   |
| 17  | AR    | 70   | THR  | CA-C-N      | 6.40  | 133.22      | 121.70   |
| 17  | AR    | 70   | THR  | C-N-CA      | 6.40  | 133.22      | 121.70   |
| 20  | AU    | 30   | GLU  | O-C-N       | -6.31 | 113.87      | 122.33   |
| 4   | AE    | 104  | ILE  | CA-C-N      | 6.30  | 133.04      | 121.70   |
| 4   | AE    | 104  | ILE  | C-N-CA      | 6.30  | 133.04      | 121.70   |
| 54  | BA    | 965  | C    | O4'-C1'-C2' | -6.28 | 101.32      | 107.60   |
| 54  | BA    | 1312 | U    | C2'-C3'-O3' | 6.25  | 118.87      | 109.50   |
| 4   | AE    | 157  | GLY  | CA-C-N      | 6.23  | 132.91      | 121.70   |
| 4   | AE    | 157  | GLY  | C-N-CA      | 6.23  | 132.91      | 121.70   |
| 54  | BA    | 643  | A    | O4'-C1'-N9  | 6.20  | 117.81      | 108.50   |
| 54  | BA    | 547  | A    | O4'-C4'-C3' | 6.20  | 110.20      | 104.00   |
| 9   | AJ    | 91   | ASP  | CA-C-N      | 6.18  | 132.83      | 121.70   |
| 9   | AJ    | 91   | ASP  | C-N-CA      | 6.18  | 132.83      | 121.70   |
| 35  | BM    | 55   | ARG  | NE-CZ-NH2   | 6.15  | 124.73      | 119.20   |
| 42  | BT    | 39   | THR  | CA-C-N      | 6.15  | 129.35      | 120.38   |
| 42  | BT    | 39   | THR  | C-N-CA      | 6.15  | 129.35      | 120.38   |
| 18  | AS    | 78   | THR  | O-C-N       | -6.15 | 114.42      | 122.59   |
| 54  | BA    | 573  | U    | C2'-C3'-O3' | 6.14  | 118.72      | 109.50   |
| 54  | BA    | 2244 | U    | O4'-C4'-C3' | 6.12  | 110.12      | 104.00   |
| 54  | BA    | 1352 | U    | O4'-C1'-N1  | 6.11  | 117.66      | 108.50   |
| 54  | BA    | 932  | U    | O4'-C1'-N1  | 6.10  | 117.35      | 108.20   |
| 54  | BA    | 2425 | A    | C2'-C3'-O3' | 6.10  | 118.65      | 109.50   |
| 54  | BA    | 481  | G    | O4'-C1'-N9  | 6.09  | 117.34      | 108.20   |
| 19  | AT    | 40   | ALA  | CA-C-N      | 6.07  | 132.62      | 121.70   |
| 19  | AT    | 40   | ALA  | C-N-CA      | 6.07  | 132.62      | 121.70   |
| 54  | BA    | 2799 | A    | O4'-C1'-C2' | -6.05 | 101.55      | 107.60   |
| 54  | BA    | 45   | G    | O4'-C4'-C3' | 6.05  | 110.05      | 104.00   |
| 1   | AB    | 10   | LYS  | O-C-N       | -6.04 | 114.56      | 122.59   |
| 54  | BA    | 804  | A    | O4'-C4'-C3' | 6.02  | 110.02      | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | AE    | 152  | VAL  | CA-C-N      | 6.02  | 132.53      | 121.70   |
| 4   | AE    | 152  | VAL  | C-N-CA      | 6.02  | 132.53      | 121.70   |
| 3   | AD    | 42   | ALA  | CA-C-N      | 6.00  | 132.51      | 121.70   |
| 3   | AD    | 42   | ALA  | C-N-CA      | 6.00  | 132.51      | 121.70   |
| 54  | BA    | 2229 | U    | C5'-C4'-C3' | -6.00 | 107.00      | 116.00   |
| 54  | BA    | 2711 | A    | C4'-C3'-O3' | 5.98  | 121.97      | 113.00   |
| 32  | BJ    | 86   | GLN  | CA-C-N      | 5.97  | 132.45      | 121.70   |
| 32  | BJ    | 86   | GLN  | C-N-CA      | 5.97  | 132.45      | 121.70   |
| 54  | BA    | 828  | U    | N1-C1'-C2'  | 5.97  | 120.96      | 112.00   |
| 10  | AK    | 124  | LYS  | CA-C-N      | 5.96  | 132.93      | 121.54   |
| 10  | AK    | 124  | LYS  | C-N-CA      | 5.96  | 132.93      | 121.54   |
| 25  | BC    | 216  | ARG  | NE-CZ-NH2   | 5.94  | 124.55      | 119.20   |
| 36  | BN    | 6    | SER  | CA-C-N      | 5.93  | 125.98      | 120.34   |
| 36  | BN    | 6    | SER  | C-N-CA      | 5.93  | 125.98      | 120.34   |
| 54  | BA    | 2389 | G    | O4'-C4'-C3' | 5.92  | 109.92      | 104.00   |
| 20  | AU    | 49   | ALA  | CA-C-N      | 5.91  | 132.34      | 121.70   |
| 20  | AU    | 49   | ALA  | C-N-CA      | 5.91  | 132.34      | 121.70   |
| 29  | BG    | 154  | GLU  | CB-CA-C     | 5.89  | 115.74      | 110.44   |
| 21  | AA    | 183  | C    | C1'-O4'-C4' | -5.88 | 104.02      | 109.90   |
| 25  | BC    | 140  | VAL  | N-CA-C      | 5.88  | 116.53      | 110.82   |
| 54  | BA    | 2667 | C    | O4'-C4'-C3' | 5.87  | 109.87      | 104.00   |
| 54  | BA    | 1126 | A    | C4'-C3'-O3' | 5.87  | 118.20      | 109.40   |
| 54  | BA    | 126  | A    | C5'-C4'-C3' | -5.86 | 107.21      | 116.00   |
| 54  | BA    | 47   | C    | O4'-C4'-C3' | 5.84  | 109.84      | 104.00   |
| 14  | AO    | 8    | ALA  | CA-C-N      | 5.83  | 132.20      | 121.70   |
| 14  | AO    | 8    | ALA  | C-N-CA      | 5.83  | 132.20      | 121.70   |
| 22  | A1    | 76   | A    | C2'-C3'-O3' | 5.81  | 118.22      | 109.50   |
| 9   | AJ    | 16   | ARG  | NE-CZ-NH2   | 5.78  | 124.40      | 119.20   |
| 21  | AA    | 626  | G    | O4'-C4'-C3' | 5.77  | 109.77      | 104.00   |
| 22  | A1    | 72   | C    | C5'-C4'-C3' | -5.77 | 106.54      | 115.20   |
| 37  | BO    | 38   | GLN  | OE1-CD-NE2  | -5.76 | 116.84      | 122.60   |
| 54  | BA    | 1236 | G    | O4'-C4'-C3' | 5.75  | 109.75      | 104.00   |
| 54  | BA    | 1847 | A    | C5'-C4'-C3' | -5.75 | 107.38      | 116.00   |
| 54  | BA    | 2580 | U    | O4'-C4'-C3' | 5.74  | 109.74      | 104.00   |
| 32  | BJ    | 86   | GLN  | O-C-N       | -5.74 | 117.77      | 123.62   |
| 54  | BA    | 747  | U    | O4'-C1'-N1  | 5.74  | 116.80      | 108.20   |
| 6   | AG    | 6    | ILE  | CA-C-N      | 5.73  | 132.01      | 121.70   |
| 6   | AG    | 6    | ILE  | C-N-CA      | 5.73  | 132.01      | 121.70   |
| 21  | AA    | 1218 | C    | O4'-C4'-C3' | 5.73  | 109.73      | 104.00   |
| 54  | BA    | 13   | A    | O4'-C4'-C3' | 5.73  | 109.73      | 104.00   |
| 54  | BA    | 2757 | A    | C5'-C4'-C3' | -5.71 | 107.43      | 116.00   |
| 21  | AA    | 366  | A    | O4'-C4'-C3' | 5.71  | 109.70      | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 926  | G    | O4'-C4'-C3' | 5.69  | 109.69      | 104.00   |
| 18  | AS    | 40   | PHE  | CA-C-N      | 5.69  | 125.80      | 119.32   |
| 18  | AS    | 40   | PHE  | C-N-CA      | 5.69  | 125.80      | 119.32   |
| 21  | AA    | 496  | A    | C1'-O4'-C4' | -5.68 | 104.22      | 109.90   |
| 54  | BA    | 1787 | A    | O4'-C4'-C3' | 5.67  | 109.67      | 104.00   |
| 25  | BC    | 12   | ARG  | NE-CZ-NH2   | 5.67  | 124.30      | 119.20   |
| 21  | AA    | 109  | A    | C1'-O4'-C4' | -5.66 | 104.04      | 109.70   |
| 21  | AA    | 1219 | A    | O4'-C4'-C3' | 5.66  | 109.66      | 104.00   |
| 21  | AA    | 1060 | U    | O3'-P-O5'   | 5.66  | 112.49      | 104.00   |
| 34  | BL    | 2    | ARG  | CA-C-N      | 5.65  | 131.87      | 121.70   |
| 34  | BL    | 2    | ARG  | C-N-CA      | 5.65  | 131.87      | 121.70   |
| 21  | AA    | 1296 | C    | O4'-C4'-C3' | 5.63  | 109.63      | 104.00   |
| 54  | BA    | 1945 | G    | O4'-C4'-C3' | 5.63  | 109.63      | 104.00   |
| 54  | BA    | 2304 | G    | O4'-C4'-C3' | 5.62  | 109.62      | 104.00   |
| 21  | AA    | 1237 | C    | O4'-C4'-C3' | 5.61  | 109.61      | 104.00   |
| 23  | A2    | 80   | C    | C1'-O4'-C4' | -5.61 | 104.29      | 109.90   |
| 54  | BA    | 1533 | C    | O4'-C4'-C3' | 5.61  | 109.61      | 104.00   |
| 54  | BA    | 850  | U    | O4'-C4'-C3' | 5.61  | 109.61      | 104.00   |
| 54  | BA    | 1085 | A    | O4'-C4'-C3' | 5.61  | 109.61      | 104.00   |
| 54  | BA    | 1977 | A    | O4'-C4'-C3' | 5.60  | 109.60      | 104.00   |
| 21  | AA    | 5    | U    | P-O3'-C3'   | 5.60  | 128.60      | 120.20   |
| 54  | BA    | 2473 | U    | O4'-C1'-N1  | 5.59  | 116.59      | 108.20   |
| 21  | AA    | 1337 | G    | O3'-P-O5'   | -5.59 | 95.62       | 104.00   |
| 30  | BH    | 84   | ALA  | CA-C-N      | 5.59  | 126.35      | 120.43   |
| 30  | BH    | 84   | ALA  | C-N-CA      | 5.59  | 126.35      | 120.43   |
| 21  | AA    | 976  | G    | O3'-P-O5'   | -5.58 | 95.63       | 104.00   |
| 21  | AA    | 1383 | C    | O4'-C4'-C3' | 5.57  | 109.57      | 104.00   |
| 54  | BA    | 456  | C    | O4'-C1'-N1  | 5.57  | 116.55      | 108.20   |
| 23  | A2    | 80   | C    | O3'-P-O5'   | 5.55  | 112.33      | 104.00   |
| 54  | BA    | 2867 | G    | O4'-C1'-N9  | 5.55  | 116.53      | 108.20   |
| 54  | BA    | 1255 | U    | O3'-P-O5'   | 5.54  | 112.31      | 104.00   |
| 41  | BS    | 90   | LYS  | CA-C-N      | 5.54  | 125.23      | 119.92   |
| 41  | BS    | 90   | LYS  | C-N-CA      | 5.54  | 125.23      | 119.92   |
| 42  | BT    | 5    | GLU  | CA-C-N      | 5.53  | 128.46      | 120.38   |
| 42  | BT    | 5    | GLU  | C-N-CA      | 5.53  | 128.46      | 120.38   |
| 21  | AA    | 382  | A    | O4'-C4'-C3' | 5.53  | 109.53      | 104.00   |
| 21  | AA    | 1150 | A    | O4'-C4'-C3' | 5.53  | 109.53      | 104.00   |
| 21  | AA    | 1255 | G    | O4'-C4'-C3' | 5.52  | 109.52      | 104.00   |
| 21  | AA    | 38   | G    | C5'-C4'-C3' | -5.52 | 107.72      | 116.00   |
| 8   | AI    | 119  | LYS  | CA-C-N      | 5.51  | 132.07      | 121.54   |
| 8   | AI    | 119  | LYS  | C-N-CA      | 5.51  | 132.07      | 121.54   |
| 21  | AA    | 413  | G    | C1'-O4'-C4' | -5.51 | 104.19      | 109.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 1197 | A    | O4'-C4'-C3' | 5.51  | 109.51      | 104.00   |
| 25  | BC    | 96   | LYS  | CA-C-N      | 5.51  | 130.21      | 121.44   |
| 25  | BC    | 96   | LYS  | C-N-CA      | 5.51  | 130.21      | 121.44   |
| 41  | BS    | 102  | HIS  | CB-CG-CD2   | -5.51 | 124.03      | 131.20   |
| 54  | BA    | 481  | G    | C1'-O4'-C4' | -5.51 | 104.19      | 109.70   |
| 54  | BA    | 1971 | U    | C1'-O4'-C4' | -5.51 | 104.19      | 109.70   |
| 3   | AD    | 37   | PRO  | CA-C-N      | 5.50  | 131.61      | 121.70   |
| 3   | AD    | 37   | PRO  | C-N-CA      | 5.50  | 131.61      | 121.70   |
| 54  | BA    | 2503 | A    | C1'-O4'-C4' | -5.49 | 104.41      | 109.90   |
| 21  | AA    | 1195 | C    | O4'-C4'-C3' | 5.48  | 109.48      | 104.00   |
| 21  | AA    | 1471 | U    | O4'-C4'-C3' | 5.48  | 109.48      | 104.00   |
| 54  | BA    | 280  | U    | O4'-C1'-N1  | 5.48  | 116.72      | 108.50   |
| 21  | AA    | 396  | C    | O3'-P-O5'   | 5.47  | 112.21      | 104.00   |
| 29  | BG    | 59   | ASP  | CA-C-N      | 5.47  | 125.91      | 119.94   |
| 29  | BG    | 59   | ASP  | C-N-CA      | 5.47  | 125.91      | 119.94   |
| 54  | BA    | 2282 | G    | C4'-C3'-O3' | 5.47  | 121.21      | 113.00   |
| 21  | AA    | 1054 | C    | C1'-O4'-C4' | -5.47 | 104.43      | 109.90   |
| 21  | AA    | 1093 | A    | C1'-O4'-C4' | -5.47 | 104.43      | 109.90   |
| 38  | BP    | 30   | TRP  | CA-C-N      | 5.47  | 131.81      | 121.97   |
| 38  | BP    | 30   | TRP  | C-N-CA      | 5.47  | 131.81      | 121.97   |
| 21  | AA    | 1014 | A    | O4'-C4'-C3' | 5.46  | 109.47      | 104.00   |
| 21  | AA    | 322  | C    | C1'-O4'-C4' | -5.46 | 104.44      | 109.90   |
| 38  | BP    | 50   | ARG  | CA-C-N      | 5.43  | 131.48      | 121.70   |
| 38  | BP    | 50   | ARG  | C-N-CA      | 5.43  | 131.48      | 121.70   |
| 9   | AJ    | 91   | ASP  | O-C-N       | -5.43 | 116.86      | 123.27   |
| 54  | BA    | 1134 | A    | O4'-C4'-C3' | 5.42  | 109.42      | 104.00   |
| 54  | BA    | 2110 | G    | C4'-C3'-O3' | 5.42  | 117.53      | 109.40   |
| 6   | AG    | 112  | ASP  | CA-C-N      | 5.41  | 131.88      | 121.54   |
| 6   | AG    | 112  | ASP  | C-N-CA      | 5.41  | 131.88      | 121.54   |
| 54  | BA    | 2425 | A    | C4'-C3'-O3' | 5.41  | 117.52      | 109.40   |
| 21  | AA    | 549  | C    | O4'-C4'-C3' | 5.39  | 109.39      | 104.00   |
| 21  | AA    | 886  | G    | O4'-C4'-C3' | 5.39  | 109.39      | 104.00   |
| 21  | AA    | 1289 | A    | O3'-P-O5'   | 5.39  | 112.08      | 104.00   |
| 21  | AA    | 1201 | A    | P-O3'-C3'   | 5.39  | 128.28      | 120.20   |
| 54  | BA    | 911  | A    | O4'-C4'-C3' | 5.39  | 109.39      | 104.00   |
| 21  | AA    | 49   | U    | O4'-C4'-C3' | 5.38  | 109.39      | 104.00   |
| 54  | BA    | 613  | A    | C1'-O4'-C4' | -5.38 | 104.52      | 109.90   |
| 54  | BA    | 1455 | G    | C5'-C4'-C3' | -5.38 | 107.93      | 116.00   |
| 54  | BA    | 1783 | A    | O4'-C4'-C3' | 5.38  | 109.38      | 104.00   |
| 54  | BA    | 2067 | G    | C2'-C3'-O3' | -5.37 | 105.64      | 113.70   |
| 49  | B0    | 24   | VAL  | CA-C-N      | 5.37  | 128.97      | 121.02   |
| 49  | B0    | 24   | VAL  | C-N-CA      | 5.37  | 128.97      | 121.02   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BA    | 482  | A    | O4'-C4'-C3' | 5.37  | 109.37      | 104.00   |
| 21  | AA    | 841  | C    | O4'-C4'-C3' | 5.37  | 109.37      | 104.00   |
| 33  | BK    | 95   | ILE  | CA-C-N      | 5.37  | 125.20      | 120.10   |
| 33  | BK    | 95   | ILE  | C-N-CA      | 5.37  | 125.20      | 120.10   |
| 54  | BA    | 2089 | C    | C1'-O4'-C4' | -5.37 | 104.53      | 109.90   |
| 54  | BA    | 613  | A    | O4'-C1'-N9  | 5.36  | 116.54      | 108.50   |
| 54  | BA    | 1263 | U    | O4'-C4'-C3' | 5.36  | 109.36      | 104.00   |
| 21  | AA    | 994  | A    | O4'-C4'-C3' | 5.36  | 109.36      | 104.00   |
| 54  | BA    | 601  | C    | C4'-C3'-C2' | -5.35 | 97.25       | 102.60   |
| 3   | AD    | 106  | PHE  | CA-C-N      | 5.35  | 126.23      | 122.33   |
| 3   | AD    | 106  | PHE  | C-N-CA      | 5.35  | 126.23      | 122.33   |
| 21  | AA    | 872  | A    | C1'-O4'-C4' | -5.35 | 104.35      | 109.70   |
| 54  | BA    | 548  | G    | O4'-C4'-C3' | 5.34  | 109.34      | 104.00   |
| 54  | BA    | 1716 | U    | C5'-C4'-C3' | -5.33 | 108.00      | 116.00   |
| 54  | BA    | 2307 | G    | O4'-C1'-N9  | 5.33  | 116.19      | 108.20   |
| 54  | BA    | 1029 | A    | C4'-C3'-C2' | -5.33 | 97.28       | 102.60   |
| 33  | BK    | 3    | GLN  | OE1-CD-NE2  | -5.31 | 117.29      | 122.60   |
| 44  | BV    | 88   | HIS  | CB-CG-CD2   | -5.30 | 124.31      | 131.20   |
| 54  | BA    | 670  | A    | C2'-C3'-O3' | 5.30  | 117.45      | 109.50   |
| 54  | BA    | 2126 | A    | O4'-C1'-N9  | 5.30  | 116.15      | 108.20   |
| 54  | BA    | 1427 | A    | C4'-C3'-O3' | 5.30  | 117.35      | 109.40   |
| 56  | B5    | 47   | ASN  | CA-C-N      | 5.29  | 131.22      | 121.70   |
| 56  | B5    | 47   | ASN  | C-N-CA      | 5.29  | 131.22      | 121.70   |
| 54  | BA    | 474  | G    | O4'-C1'-N9  | 5.28  | 116.12      | 108.20   |
| 54  | BA    | 46   | G    | O4'-C4'-C3' | 5.28  | 109.28      | 104.00   |
| 54  | BA    | 1907 | G    | C5'-C4'-C3' | -5.28 | 108.09      | 116.00   |
| 54  | BA    | 2058 | A    | O4'-C4'-C3' | 5.28  | 109.28      | 104.00   |
| 31  | BI    | 21   | PRO  | N-CA-C      | 5.27  | 117.13      | 110.70   |
| 27  | BE    | 43   | THR  | CA-C-N      | 5.27  | 128.33      | 120.90   |
| 27  | BE    | 43   | THR  | C-N-CA      | 5.27  | 128.33      | 120.90   |
| 54  | BA    | 1459 | G    | O4'-C1'-N9  | 5.27  | 116.11      | 108.20   |
| 54  | BA    | 2438 | U    | O4'-C4'-C3' | 5.27  | 109.27      | 104.00   |
| 30  | BH    | 40   | THR  | CA-C-N      | 5.26  | 127.59      | 120.38   |
| 30  | BH    | 40   | THR  | C-N-CA      | 5.26  | 127.59      | 120.38   |
| 21  | AA    | 1342 | C    | C2'-C3'-O3' | 5.26  | 121.58      | 113.70   |
| 29  | BG    | 172  | GLU  | CA-C-N      | 5.25  | 131.15      | 121.70   |
| 29  | BG    | 172  | GLU  | C-N-CA      | 5.25  | 131.15      | 121.70   |
| 54  | BA    | 2054 | A    | O4'-C4'-C3' | 5.25  | 109.25      | 104.00   |
| 21  | AA    | 436  | C    | C5'-C4'-C3' | -5.25 | 108.13      | 116.00   |
| 24  | A3    | 19   | G    | O4'-C4'-C3' | 5.25  | 109.25      | 104.00   |
| 54  | BA    | 572  | A    | O4'-C4'-C3' | 5.24  | 109.24      | 104.00   |
| 8   | AI    | 112  | ARG  | CA-C-N      | 5.24  | 129.16      | 120.94   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8   | AI    | 112  | ARG  | C-N-CA      | 5.24  | 129.16      | 120.94   |
| 54  | BA    | 1805 | A    | C4'-C3'-C2' | -5.24 | 97.36       | 102.60   |
| 54  | BA    | 1929 | G    | O4'-C1'-N9  | 5.24  | 116.06      | 108.20   |
| 14  | AO    | 50   | HIS  | CB-CG-CD2   | -5.24 | 124.39      | 131.20   |
| 21  | AA    | 124  | C    | O4'-C4'-C3' | 5.23  | 109.23      | 104.00   |
| 54  | BA    | 998  | C    | C4'-C3'-C2' | -5.23 | 97.37       | 102.60   |
| 54  | BA    | 443  | A    | C1'-O4'-C4' | -5.22 | 104.47      | 109.70   |
| 54  | BA    | 1387 | A    | O4'-C1'-N9  | 5.22  | 116.02      | 108.20   |
| 54  | BA    | 1933 | G    | C4'-C3'-C2' | -5.21 | 97.39       | 102.60   |
| 54  | BA    | 1024 | G    | C2'-C3'-O3' | -5.21 | 105.89      | 113.70   |
| 17  | AR    | 73   | HIS  | CB-CG-CD2   | -5.21 | 124.43      | 131.20   |
| 3   | AD    | 36   | ALA  | CA-C-N      | 5.21  | 124.71      | 119.19   |
| 3   | AD    | 36   | ALA  | C-N-CA      | 5.21  | 124.71      | 119.19   |
| 21  | AA    | 1101 | A    | P-O3'-C3'   | 5.20  | 128.00      | 120.20   |
| 11  | AL    | 46   | SER  | CA-C-N      | 5.20  | 131.47      | 121.54   |
| 11  | AL    | 46   | SER  | C-N-CA      | 5.20  | 131.47      | 121.54   |
| 29  | BG    | 173  | ALA  | CA-C-N      | 5.20  | 131.06      | 121.70   |
| 29  | BG    | 173  | ALA  | C-N-CA      | 5.20  | 131.06      | 121.70   |
| 54  | BA    | 427  | U    | C2'-C3'-O3' | -5.20 | 105.91      | 113.70   |
| 21  | AA    | 1344 | C    | O4'-C4'-C3' | 5.19  | 109.19      | 104.00   |
| 54  | BA    | 2712 | C    | O4'-C4'-C3' | 5.19  | 109.19      | 104.00   |
| 54  | BA    | 346  | A    | O4'-C1'-C2' | -5.18 | 102.42      | 107.60   |
| 54  | BA    | 127  | A    | O4'-C4'-C3' | 5.18  | 109.18      | 104.00   |
| 19  | AT    | 67   | HIS  | CB-CG-CD2   | -5.18 | 124.47      | 131.20   |
| 54  | BA    | 1236 | G    | C4'-C3'-O3' | -5.18 | 105.23      | 113.00   |
| 54  | BA    | 2503 | A    | O4'-C1'-N9  | 5.18  | 116.27      | 108.50   |
| 24  | A3    | 36   | A    | C1'-O4'-C4' | -5.18 | 104.72      | 109.90   |
| 7   | AH    | 52   | GLY  | CA-C-N      | 5.17  | 131.01      | 121.70   |
| 7   | AH    | 52   | GLY  | C-N-CA      | 5.17  | 131.01      | 121.70   |
| 15  | AP    | 79   | ASN  | CA-C-N      | 5.17  | 131.00      | 121.70   |
| 15  | AP    | 79   | ASN  | C-N-CA      | 5.17  | 131.00      | 121.70   |
| 54  | BA    | 164  | C    | C4'-C3'-C2' | -5.15 | 97.45       | 102.60   |
| 54  | BA    | 1938 | A    | O4'-C1'-N9  | 5.15  | 115.92      | 108.20   |
| 21  | AA    | 834  | U    | C5'-C4'-C3' | -5.14 | 108.28      | 116.00   |
| 21  | AA    | 285  | C    | O4'-C4'-C3' | 5.14  | 109.14      | 104.00   |
| 11  | AL    | 71   | HIS  | CB-CG-CD2   | -5.14 | 124.52      | 131.20   |
| 54  | BA    | 1161 | C    | C4'-C3'-C2' | -5.14 | 97.46       | 102.60   |
| 54  | BA    | 1154 | G    | C2'-C3'-O3' | -5.13 | 106.00      | 113.70   |
| 54  | BA    | 1936 | A    | O4'-C4'-C3' | 5.13  | 109.13      | 104.00   |
| 13  | AN    | 100  | SER  | CA-C-N      | 5.13  | 130.94      | 121.70   |
| 13  | AN    | 100  | SER  | C-N-CA      | 5.13  | 130.94      | 121.70   |
| 21  | AA    | 1267 | C    | O4'-C4'-C3' | 5.13  | 109.13      | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 1308 | U    | C4'-C3'-O3' | 5.13  | 120.69      | 113.00   |
| 24  | A3    | 59   | A    | O4'-C4'-C3' | 5.13  | 109.13      | 104.00   |
| 54  | BA    | 1067 | A    | O4'-C1'-N9  | 5.12  | 115.89      | 108.20   |
| 21  | AA    | 349  | A    | C5'-C4'-C3' | -5.12 | 108.31      | 116.00   |
| 43  | BU    | 71   | ILE  | CA-C-N      | 5.12  | 128.12      | 120.95   |
| 43  | BU    | 71   | ILE  | C-N-CA      | 5.12  | 128.12      | 120.95   |
| 21  | AA    | 738  | C    | C5'-C4'-C3' | -5.12 | 108.32      | 116.00   |
| 54  | BA    | 1501 | G    | C5'-C4'-C3' | -5.12 | 108.32      | 116.00   |
| 24  | A3    | 73   | A    | P-O5'-C5'   | 5.12  | 128.58      | 120.90   |
| 54  | BA    | 1292 | G    | O4'-C4'-C3' | 5.11  | 109.11      | 104.00   |
| 6   | AG    | 4    | ARG  | O-C-N       | -5.11 | 117.13      | 123.36   |
| 21  | AA    | 869  | G    | O4'-C4'-C3' | 5.11  | 109.11      | 104.00   |
| 54  | BA    | 532  | A    | O4'-C1'-N9  | 5.11  | 115.86      | 108.20   |
| 21  | AA    | 1087 | G    | O4'-C4'-C3' | 5.10  | 109.10      | 104.00   |
| 54  | BA    | 1938 | A    | C1'-O4'-C4' | -5.10 | 104.60      | 109.70   |
| 54  | BA    | 2322 | A    | O4'-C4'-C3' | 5.09  | 109.09      | 104.00   |
| 56  | B5    | 47   | ASN  | O-C-N       | -5.09 | 117.31      | 123.27   |
| 21  | AA    | 70   | U    | O3'-P-O5'   | -5.09 | 96.36       | 104.00   |
| 21  | AA    | 184  | G    | O4'-C4'-C3' | 5.09  | 109.09      | 104.00   |
| 27  | BE    | 100  | MET  | CA-C-N      | 5.09  | 127.10      | 120.28   |
| 27  | BE    | 100  | MET  | C-N-CA      | 5.09  | 127.10      | 120.28   |
| 54  | BA    | 1158 | C    | O4'-C4'-C3' | 5.09  | 109.09      | 104.00   |
| 21  | AA    | 46   | G    | O4'-C4'-C3' | 5.09  | 109.09      | 104.00   |
| 21  | AA    | 673  | A    | C5'-C4'-C3' | -5.09 | 108.37      | 116.00   |
| 54  | BA    | 1434 | A    | C4'-C3'-C2' | -5.08 | 97.52       | 102.60   |
| 21  | AA    | 1233 | G    | O4'-C4'-C3' | 5.08  | 109.08      | 104.00   |
| 54  | BA    | 309  | A    | O4'-C4'-C3' | 5.08  | 109.08      | 104.00   |
| 3   | AD    | 184  | LYS  | CA-C-N      | 5.07  | 125.06      | 119.89   |
| 3   | AD    | 184  | LYS  | C-N-CA      | 5.07  | 125.06      | 119.89   |
| 55  | BB    | 87   | U    | O4'-C1'-N1  | 5.07  | 115.80      | 108.20   |
| 21  | AA    | 474  | G    | O4'-C4'-C3' | 5.06  | 109.06      | 104.00   |
| 54  | BA    | 1635 | A    | O4'-C4'-C3' | 5.06  | 109.06      | 104.00   |
| 21  | AA    | 724  | G    | C5'-C4'-C3' | -5.06 | 108.41      | 116.00   |
| 24  | A3    | 15   | G    | O4'-C4'-C3' | 5.06  | 109.06      | 104.00   |
| 39  | BQ    | 1    | ALA  | CA-C-N      | 5.06  | 130.80      | 121.70   |
| 39  | BQ    | 1    | ALA  | C-N-CA      | 5.06  | 130.80      | 121.70   |
| 54  | BA    | 1010 | A    | O4'-C4'-C3' | 5.05  | 109.05      | 104.00   |
| 3   | AD    | 79   | ALA  | CA-C-N      | 5.05  | 130.88      | 122.20   |
| 3   | AD    | 79   | ALA  | C-N-CA      | 5.05  | 130.88      | 122.20   |
| 21  | AA    | 864  | A    | O4'-C4'-C3' | 5.04  | 109.05      | 104.00   |
| 54  | BA    | 333  | G    | O4'-C4'-C3' | 5.04  | 109.04      | 104.00   |
| 9   | AJ    | 101  | SER  | CA-C-N      | 5.04  | 130.78      | 121.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9   | AJ    | 101  | SER  | C-N-CA      | 5.04  | 130.78      | 121.70   |
| 21  | AA    | 1308 | U    | C3'-C2'-C1' | -5.04 | 96.26       | 101.30   |
| 54  | BA    | 841  | G    | C4'-C3'-C2' | -5.04 | 97.56       | 102.60   |
| 54  | BA    | 1609 | A    | C1'-O4'-C4' | -5.04 | 104.86      | 109.90   |
| 20  | AU    | 47   | ALA  | CA-C-N      | 5.04  | 130.77      | 121.70   |
| 20  | AU    | 47   | ALA  | C-N-CA      | 5.04  | 130.77      | 121.70   |
| 54  | BA    | 781  | A    | O3'-P-O5'   | -5.04 | 96.44       | 104.00   |
| 40  | BR    | 66   | HIS  | CB-CG-CD2   | -5.04 | 124.66      | 131.20   |
| 54  | BA    | 562  | U    | O4'-C4'-C3' | 5.03  | 109.03      | 104.00   |
| 21  | AA    | 1188 | A    | O4'-C4'-C3' | 5.03  | 109.03      | 104.00   |
| 54  | BA    | 1110 | G    | O4'-C4'-C3' | 5.03  | 109.03      | 104.00   |
| 52  | B3    | 25   | HIS  | CB-CG-CD2   | -5.03 | 124.67      | 131.20   |
| 25  | BC    | 229  | HIS  | CB-CG-CD2   | -5.02 | 124.67      | 131.20   |
| 54  | BA    | 989  | G    | C3'-C2'-C1' | 5.02  | 106.32      | 101.30   |
| 21  | AA    | 1421 | G    | C5'-C4'-C3' | -5.02 | 108.47      | 116.00   |
| 10  | AK    | 122  | PRO  | CA-C-N      | 5.01  | 125.01      | 119.90   |
| 10  | AK    | 122  | PRO  | C-N-CA      | 5.01  | 125.01      | 119.90   |
| 37  | BO    | 81   | ARG  | NH1-CZ-NH2  | -5.01 | 112.79      | 119.30   |
| 54  | BA    | 26   | G    | O4'-C4'-C3' | 5.01  | 109.01      | 104.00   |
| 54  | BA    | 2565 | A    | O4'-C4'-C3' | 5.01  | 109.01      | 104.00   |
| 31  | BI    | 110  | GLN  | OE1-CD-NE2  | -5.01 | 117.59      | 122.60   |
| 54  | BA    | 1335 | C    | O4'-C4'-C3' | 5.01  | 109.01      | 104.00   |
| 21  | AA    | 1336 | C    | O3'-P-O5'   | -5.00 | 96.49       | 104.00   |
| 21  | AA    | 847  | G    | O4'-C4'-C3' | 5.00  | 109.00      | 104.00   |

There are no chirality outliers.

All (1158) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 22  | A1    | 11  | C    | Sidechain |
| 22  | A1    | 15  | G    | Sidechain |
| 22  | A1    | 18  | G    | Sidechain |
| 22  | A1    | 19  | G    | Sidechain |
| 22  | A1    | 2   | G    | Sidechain |
| 22  | A1    | 25  | C    | Sidechain |
| 22  | A1    | 28  | C    | Sidechain |
| 22  | A1    | 29  | U    | Sidechain |
| 22  | A1    | 30  | C    | Sidechain |
| 22  | A1    | 33  | U    | Sidechain |
| 22  | A1    | 43  | G    | Sidechain |
| 22  | A1    | 58  | A    | Sidechain |
| 22  | A1    | 6   | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 22  | A1    | 65   | C    | Sidechain |
| 22  | A1    | 66   | A    | Sidechain |
| 22  | A1    | 67   | U    | Sidechain |
| 22  | A1    | 70   | C    | Sidechain |
| 22  | A1    | 73   | A    | Sidechain |
| 22  | A1    | 74   | C    | Sidechain |
| 22  | A1    | 76   | A    | Sidechain |
| 22  | A1    | 8    | U    | Sidechain |
| 23  | A2    | 80   | C    | Sidechain |
| 23  | A2    | 83   | U    | Sidechain |
| 23  | A2    | 84   | G    | Sidechain |
| 23  | A2    | 85   | G    | Sidechain |
| 23  | A2    | 92   | U    | Sidechain |
| 24  | A3    | 11   | A    | Sidechain |
| 24  | A3    | 2    | G    | Sidechain |
| 24  | A3    | 34   | U    | Sidechain |
| 24  | A3    | 46   | G    | Sidechain |
| 24  | A3    | 54   | G    | Sidechain |
| 24  | A3    | 60   | A    | Sidechain |
| 24  | A3    | 66   | C    | Sidechain |
| 21  | AA    | 10   | A    | Sidechain |
| 21  | AA    | 1000 | A    | Sidechain |
| 21  | AA    | 1012 | A    | Sidechain |
| 21  | AA    | 1013 | G    | Sidechain |
| 21  | AA    | 1019 | A    | Sidechain |
| 21  | AA    | 1021 | A    | Sidechain |
| 21  | AA    | 1025 | U    | Sidechain |
| 21  | AA    | 1033 | G    | Sidechain |
| 21  | AA    | 1048 | G    | Sidechain |
| 21  | AA    | 1049 | U    | Sidechain |
| 21  | AA    | 1052 | U    | Sidechain |
| 21  | AA    | 1055 | A    | Sidechain |
| 21  | AA    | 1057 | G    | Sidechain |
| 21  | AA    | 1058 | G    | Sidechain |
| 21  | AA    | 1060 | U    | Sidechain |
| 21  | AA    | 1061 | G    | Sidechain |
| 21  | AA    | 1064 | G    | Sidechain |
| 21  | AA    | 1069 | C    | Sidechain |
| 21  | AA    | 1073 | U    | Sidechain |
| 21  | AA    | 1077 | G    | Sidechain |
| 21  | AA    | 108  | G    | Sidechain |
| 21  | AA    | 1080 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 21  | AA    | 1083 | U    | Sidechain |
| 21  | AA    | 1084 | G    | Sidechain |
| 21  | AA    | 1085 | U    | Sidechain |
| 21  | AA    | 109  | A    | Sidechain |
| 21  | AA    | 1101 | A    | Sidechain |
| 21  | AA    | 1107 | C    | Sidechain |
| 21  | AA    | 1117 | A    | Sidechain |
| 21  | AA    | 1125 | U    | Sidechain |
| 21  | AA    | 1128 | C    | Sidechain |
| 21  | AA    | 1129 | C    | Sidechain |
| 21  | AA    | 1131 | G    | Sidechain |
| 21  | AA    | 1139 | G    | Sidechain |
| 21  | AA    | 114  | U    | Sidechain |
| 21  | AA    | 1141 | C    | Sidechain |
| 21  | AA    | 1147 | C    | Sidechain |
| 21  | AA    | 1153 | G    | Sidechain |
| 21  | AA    | 1158 | C    | Sidechain |
| 21  | AA    | 1161 | C    | Sidechain |
| 21  | AA    | 1167 | A    | Sidechain |
| 21  | AA    | 1178 | G    | Sidechain |
| 21  | AA    | 1184 | G    | Sidechain |
| 21  | AA    | 1193 | G    | Sidechain |
| 21  | AA    | 1195 | C    | Sidechain |
| 21  | AA    | 12   | U    | Sidechain |
| 21  | AA    | 1202 | U    | Sidechain |
| 21  | AA    | 1204 | A    | Sidechain |
| 21  | AA    | 121  | U    | Sidechain |
| 21  | AA    | 1211 | U    | Sidechain |
| 21  | AA    | 1212 | U    | Sidechain |
| 21  | AA    | 1225 | A    | Sidechain |
| 21  | AA    | 1226 | C    | Sidechain |
| 21  | AA    | 1227 | A    | Sidechain |
| 21  | AA    | 1228 | C    | Sidechain |
| 21  | AA    | 123  | U    | Sidechain |
| 21  | AA    | 1234 | C    | Sidechain |
| 21  | AA    | 125  | U    | Sidechain |
| 21  | AA    | 1256 | A    | Sidechain |
| 21  | AA    | 1264 | U    | Sidechain |
| 21  | AA    | 1266 | G    | Sidechain |
| 21  | AA    | 1276 | G    | Sidechain |
| 21  | AA    | 1279 | G    | Sidechain |
| 21  | AA    | 1285 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 21  | AA    | 1289 | A    | Sidechain |
| 21  | AA    | 129  | A    | Sidechain |
| 21  | AA    | 1297 | G    | Sidechain |
| 21  | AA    | 1298 | U    | Sidechain |
| 21  | AA    | 1300 | G    | Sidechain |
| 21  | AA    | 1301 | U    | Sidechain |
| 21  | AA    | 1303 | C    | Sidechain |
| 21  | AA    | 1304 | G    | Sidechain |
| 21  | AA    | 1309 | G    | Sidechain |
| 21  | AA    | 1316 | G    | Sidechain |
| 21  | AA    | 1320 | C    | Sidechain |
| 21  | AA    | 1321 | U    | Sidechain |
| 21  | AA    | 1324 | A    | Sidechain |
| 21  | AA    | 1326 | U    | Sidechain |
| 21  | AA    | 1328 | C    | Sidechain |
| 21  | AA    | 1331 | G    | Sidechain |
| 21  | AA    | 1335 | U    | Sidechain |
| 21  | AA    | 1336 | C    | Sidechain |
| 21  | AA    | 1337 | G    | Sidechain |
| 21  | AA    | 1339 | A    | Sidechain |
| 21  | AA    | 1342 | C    | Sidechain |
| 21  | AA    | 1343 | G    | Sidechain |
| 21  | AA    | 1356 | G    | Sidechain |
| 21  | AA    | 1357 | A    | Sidechain |
| 21  | AA    | 1359 | C    | Sidechain |
| 21  | AA    | 1361 | G    | Sidechain |
| 21  | AA    | 1366 | C    | Sidechain |
| 21  | AA    | 1386 | G    | Sidechain |
| 21  | AA    | 1387 | G    | Sidechain |
| 21  | AA    | 1390 | U    | Sidechain |
| 21  | AA    | 1392 | G    | Sidechain |
| 21  | AA    | 1397 | C    | Sidechain |
| 21  | AA    | 1398 | A    | Sidechain |
| 21  | AA    | 1399 | C    | Sidechain |
| 21  | AA    | 140  | U    | Sidechain |
| 21  | AA    | 1400 | C    | Sidechain |
| 21  | AA    | 1405 | G    | Sidechain |
| 21  | AA    | 1406 | U    | Sidechain |
| 21  | AA    | 1432 | G    | Sidechain |
| 21  | AA    | 1435 | G    | Sidechain |
| 21  | AA    | 1436 | U    | Sidechain |
| 21  | AA    | 1438 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 21  | AA    | 1439 | G    | Sidechain |
| 21  | AA    | 1441 | A    | Sidechain |
| 21  | AA    | 1442 | G    | Sidechain |
| 21  | AA    | 1448 | C    | Sidechain |
| 21  | AA    | 1452 | C    | Sidechain |
| 21  | AA    | 1459 | G    | Sidechain |
| 21  | AA    | 1465 | A    | Sidechain |
| 21  | AA    | 1473 | G    | Sidechain |
| 21  | AA    | 1478 | U    | Sidechain |
| 21  | AA    | 148  | G    | Sidechain |
| 21  | AA    | 1484 | C    | Sidechain |
| 21  | AA    | 1491 | G    | Sidechain |
| 21  | AA    | 1493 | A    | Sidechain |
| 21  | AA    | 1494 | G    | Sidechain |
| 21  | AA    | 1495 | U    | Sidechain |
| 21  | AA    | 1498 | U    | Sidechain |
| 21  | AA    | 1504 | G    | Sidechain |
| 21  | AA    | 1512 | U    | Sidechain |
| 21  | AA    | 1514 | G    | Sidechain |
| 21  | AA    | 1516 | G    | Sidechain |
| 21  | AA    | 1517 | G    | Sidechain |
| 21  | AA    | 1519 | A    | Sidechain |
| 21  | AA    | 152  | A    | Sidechain |
| 21  | AA    | 1523 | G    | Sidechain |
| 21  | AA    | 153  | C    | Sidechain |
| 21  | AA    | 159  | G    | Sidechain |
| 21  | AA    | 163  | C    | Sidechain |
| 21  | AA    | 168  | G    | Sidechain |
| 21  | AA    | 173  | U    | Sidechain |
| 21  | AA    | 175  | C    | Sidechain |
| 21  | AA    | 184  | G    | Sidechain |
| 21  | AA    | 187  | G    | Sidechain |
| 21  | AA    | 195  | A    | Sidechain |
| 21  | AA    | 197  | A    | Sidechain |
| 21  | AA    | 198  | G    | Sidechain |
| 21  | AA    | 20   | U    | Sidechain |
| 21  | AA    | 200  | G    | Sidechain |
| 21  | AA    | 201  | G    | Sidechain |
| 21  | AA    | 204  | G    | Sidechain |
| 21  | AA    | 206  | C    | Sidechain |
| 21  | AA    | 208  | U    | Sidechain |
| 21  | AA    | 211  | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 21  | AA    | 215 | C    | Sidechain |
| 21  | AA    | 223 | A    | Sidechain |
| 21  | AA    | 236 | A    | Sidechain |
| 21  | AA    | 238 | A    | Sidechain |
| 21  | AA    | 239 | U    | Sidechain |
| 21  | AA    | 240 | G    | Sidechain |
| 21  | AA    | 241 | G    | Sidechain |
| 21  | AA    | 254 | G    | Sidechain |
| 21  | AA    | 257 | G    | Sidechain |
| 21  | AA    | 26  | A    | Sidechain |
| 21  | AA    | 263 | A    | Sidechain |
| 21  | AA    | 266 | G    | Sidechain |
| 21  | AA    | 282 | A    | Sidechain |
| 21  | AA    | 284 | C    | Sidechain |
| 21  | AA    | 29  | U    | Sidechain |
| 21  | AA    | 292 | G    | Sidechain |
| 21  | AA    | 294 | U    | Sidechain |
| 21  | AA    | 295 | C    | Sidechain |
| 21  | AA    | 296 | U    | Sidechain |
| 21  | AA    | 298 | A    | Sidechain |
| 21  | AA    | 299 | G    | Sidechain |
| 21  | AA    | 304 | U    | Sidechain |
| 21  | AA    | 305 | G    | Sidechain |
| 21  | AA    | 308 | C    | Sidechain |
| 21  | AA    | 31  | G    | Sidechain |
| 21  | AA    | 314 | C    | Sidechain |
| 21  | AA    | 315 | A    | Sidechain |
| 21  | AA    | 316 | C    | Sidechain |
| 21  | AA    | 317 | U    | Sidechain |
| 21  | AA    | 324 | G    | Sidechain |
| 21  | AA    | 328 | C    | Sidechain |
| 21  | AA    | 331 | G    | Sidechain |
| 21  | AA    | 333 | U    | Sidechain |
| 21  | AA    | 336 | A    | Sidechain |
| 21  | AA    | 337 | G    | Sidechain |
| 21  | AA    | 340 | U    | Sidechain |
| 21  | AA    | 346 | G    | Sidechain |
| 21  | AA    | 349 | A    | Sidechain |
| 21  | AA    | 359 | G    | Sidechain |
| 21  | AA    | 36  | C    | Sidechain |
| 21  | AA    | 362 | G    | Sidechain |
| 21  | AA    | 363 | A    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 21  | AA    | 368 | U    | Sidechain |
| 21  | AA    | 373 | A    | Sidechain |
| 21  | AA    | 376 | G    | Sidechain |
| 21  | AA    | 377 | G    | Sidechain |
| 21  | AA    | 380 | G    | Sidechain |
| 21  | AA    | 381 | C    | Sidechain |
| 21  | AA    | 382 | A    | Sidechain |
| 21  | AA    | 383 | A    | Sidechain |
| 21  | AA    | 384 | G    | Sidechain |
| 21  | AA    | 388 | G    | Sidechain |
| 21  | AA    | 391 | G    | Sidechain |
| 21  | AA    | 397 | A    | Sidechain |
| 21  | AA    | 403 | C    | Sidechain |
| 21  | AA    | 404 | G    | Sidechain |
| 21  | AA    | 408 | A    | Sidechain |
| 21  | AA    | 409 | U    | Sidechain |
| 21  | AA    | 412 | A    | Sidechain |
| 21  | AA    | 413 | G    | Sidechain |
| 21  | AA    | 421 | U    | Sidechain |
| 21  | AA    | 423 | G    | Sidechain |
| 21  | AA    | 425 | G    | Sidechain |
| 21  | AA    | 427 | U    | Sidechain |
| 21  | AA    | 428 | G    | Sidechain |
| 21  | AA    | 429 | U    | Sidechain |
| 21  | AA    | 430 | A    | Sidechain |
| 21  | AA    | 436 | C    | Sidechain |
| 21  | AA    | 442 | G    | Sidechain |
| 21  | AA    | 446 | G    | Sidechain |
| 21  | AA    | 448 | A    | Sidechain |
| 21  | AA    | 450 | G    | Sidechain |
| 21  | AA    | 453 | G    | Sidechain |
| 21  | AA    | 454 | G    | Sidechain |
| 21  | AA    | 459 | A    | Sidechain |
| 21  | AA    | 461 | A    | Sidechain |
| 21  | AA    | 464 | U    | Sidechain |
| 21  | AA    | 466 | A    | Sidechain |
| 21  | AA    | 467 | U    | Sidechain |
| 21  | AA    | 47  | C    | Sidechain |
| 21  | AA    | 476 | U    | Sidechain |
| 21  | AA    | 480 | U    | Sidechain |
| 21  | AA    | 481 | G    | Sidechain |
| 21  | AA    | 483 | C    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 21  | AA    | 487 | A    | Sidechain |
| 21  | AA    | 494 | G    | Sidechain |
| 21  | AA    | 499 | A    | Sidechain |
| 21  | AA    | 5   | U    | Sidechain |
| 21  | AA    | 50  | A    | Sidechain |
| 21  | AA    | 500 | G    | Sidechain |
| 21  | AA    | 503 | C    | Sidechain |
| 21  | AA    | 504 | C    | Sidechain |
| 21  | AA    | 505 | G    | Sidechain |
| 21  | AA    | 506 | G    | Sidechain |
| 21  | AA    | 513 | C    | Sidechain |
| 21  | AA    | 517 | G    | Sidechain |
| 21  | AA    | 519 | C    | Sidechain |
| 21  | AA    | 524 | G    | Sidechain |
| 21  | AA    | 530 | G    | Sidechain |
| 21  | AA    | 535 | A    | Sidechain |
| 21  | AA    | 536 | C    | Sidechain |
| 21  | AA    | 537 | G    | Sidechain |
| 21  | AA    | 538 | G    | Sidechain |
| 21  | AA    | 540 | G    | Sidechain |
| 21  | AA    | 558 | G    | Sidechain |
| 21  | AA    | 564 | C    | Sidechain |
| 21  | AA    | 568 | G    | Sidechain |
| 21  | AA    | 572 | A    | Sidechain |
| 21  | AA    | 575 | G    | Sidechain |
| 21  | AA    | 583 | A    | Sidechain |
| 21  | AA    | 597 | G    | Sidechain |
| 21  | AA    | 60  | A    | Sidechain |
| 21  | AA    | 600 | A    | Sidechain |
| 21  | AA    | 604 | G    | Sidechain |
| 21  | AA    | 608 | A    | Sidechain |
| 21  | AA    | 61  | G    | Sidechain |
| 21  | AA    | 610 | U    | Sidechain |
| 21  | AA    | 612 | C    | Sidechain |
| 21  | AA    | 613 | C    | Sidechain |
| 21  | AA    | 614 | C    | Sidechain |
| 21  | AA    | 617 | G    | Sidechain |
| 21  | AA    | 618 | C    | Sidechain |
| 21  | AA    | 620 | C    | Sidechain |
| 21  | AA    | 621 | A    | Sidechain |
| 21  | AA    | 623 | C    | Sidechain |
| 21  | AA    | 626 | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 21  | AA    | 628 | G    | Sidechain |
| 21  | AA    | 633 | G    | Sidechain |
| 21  | AA    | 640 | A    | Sidechain |
| 21  | AA    | 641 | U    | Sidechain |
| 21  | AA    | 642 | A    | Sidechain |
| 21  | AA    | 646 | G    | Sidechain |
| 21  | AA    | 652 | U    | Sidechain |
| 21  | AA    | 662 | U    | Sidechain |
| 21  | AA    | 672 | U    | Sidechain |
| 21  | AA    | 675 | A    | Sidechain |
| 21  | AA    | 676 | A    | Sidechain |
| 21  | AA    | 677 | U    | Sidechain |
| 21  | AA    | 678 | U    | Sidechain |
| 21  | AA    | 682 | G    | Sidechain |
| 21  | AA    | 69  | G    | Sidechain |
| 21  | AA    | 690 | G    | Sidechain |
| 21  | AA    | 691 | G    | Sidechain |
| 21  | AA    | 695 | A    | Sidechain |
| 21  | AA    | 698 | G    | Sidechain |
| 21  | AA    | 700 | G    | Sidechain |
| 21  | AA    | 703 | G    | Sidechain |
| 21  | AA    | 710 | G    | Sidechain |
| 21  | AA    | 714 | G    | Sidechain |
| 21  | AA    | 715 | A    | Sidechain |
| 21  | AA    | 717 | U    | Sidechain |
| 21  | AA    | 727 | G    | Sidechain |
| 21  | AA    | 739 | C    | Sidechain |
| 21  | AA    | 740 | U    | Sidechain |
| 21  | AA    | 741 | G    | Sidechain |
| 21  | AA    | 752 | G    | Sidechain |
| 21  | AA    | 754 | C    | Sidechain |
| 21  | AA    | 76  | G    | Sidechain |
| 21  | AA    | 760 | G    | Sidechain |
| 21  | AA    | 763 | G    | Sidechain |
| 21  | AA    | 764 | C    | Sidechain |
| 21  | AA    | 766 | A    | Sidechain |
| 21  | AA    | 771 | G    | Sidechain |
| 21  | AA    | 79  | G    | Sidechain |
| 21  | AA    | 790 | A    | Sidechain |
| 21  | AA    | 795 | C    | Sidechain |
| 21  | AA    | 798 | U    | Sidechain |
| 21  | AA    | 803 | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 21  | AA    | 804 | U    | Sidechain |
| 21  | AA    | 805 | C    | Sidechain |
| 21  | AA    | 811 | C    | Sidechain |
| 21  | AA    | 816 | A    | Sidechain |
| 21  | AA    | 819 | A    | Sidechain |
| 21  | AA    | 824 | G    | Sidechain |
| 21  | AA    | 826 | C    | Sidechain |
| 21  | AA    | 827 | U    | Sidechain |
| 21  | AA    | 829 | G    | Sidechain |
| 21  | AA    | 833 | G    | Sidechain |
| 21  | AA    | 836 | G    | Sidechain |
| 21  | AA    | 838 | G    | Sidechain |
| 21  | AA    | 840 | C    | Sidechain |
| 21  | AA    | 842 | U    | Sidechain |
| 21  | AA    | 844 | G    | Sidechain |
| 21  | AA    | 846 | G    | Sidechain |
| 21  | AA    | 865 | A    | Sidechain |
| 21  | AA    | 873 | A    | Sidechain |
| 21  | AA    | 875 | U    | Sidechain |
| 21  | AA    | 881 | G    | Sidechain |
| 21  | AA    | 884 | U    | Sidechain |
| 21  | AA    | 887 | G    | Sidechain |
| 21  | AA    | 891 | U    | Sidechain |
| 21  | AA    | 895 | G    | Sidechain |
| 21  | AA    | 898 | G    | Sidechain |
| 21  | AA    | 899 | C    | Sidechain |
| 21  | AA    | 90  | C    | Sidechain |
| 21  | AA    | 900 | A    | Sidechain |
| 21  | AA    | 903 | G    | Sidechain |
| 21  | AA    | 904 | U    | Sidechain |
| 21  | AA    | 905 | U    | Sidechain |
| 21  | AA    | 909 | A    | Sidechain |
| 21  | AA    | 917 | G    | Sidechain |
| 21  | AA    | 926 | G    | Sidechain |
| 21  | AA    | 928 | G    | Sidechain |
| 21  | AA    | 931 | C    | Sidechain |
| 21  | AA    | 933 | G    | Sidechain |
| 21  | AA    | 94  | G    | Sidechain |
| 21  | AA    | 943 | U    | Sidechain |
| 21  | AA    | 944 | G    | Sidechain |
| 21  | AA    | 947 | G    | Sidechain |
| 21  | AA    | 949 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 21  | AA    | 954  | G    | Sidechain |
| 21  | AA    | 957  | U    | Sidechain |
| 21  | AA    | 961  | U    | Sidechain |
| 21  | AA    | 966  | G    | Sidechain |
| 21  | AA    | 97   | G    | Sidechain |
| 21  | AA    | 978  | A    | Sidechain |
| 21  | AA    | 981  | U    | Sidechain |
| 21  | AA    | 982  | U    | Sidechain |
| 21  | AA    | 986  | U    | Sidechain |
| 21  | AA    | 988  | G    | Sidechain |
| 21  | AA    | 990  | C    | Sidechain |
| 21  | AA    | 991  | U    | Sidechain |
| 21  | AA    | 994  | A    | Sidechain |
| 21  | AA    | 999  | C    | Sidechain |
| 3   | AD    | 204  | SER  | Mainchain |
| 8   | AI    | 105  | ARG  | Sidechain |
| 14  | AO    | 87   | ARG  | Sidechain |
| 54  | BA    | 1000 | A    | Sidechain |
| 54  | BA    | 101  | A    | Sidechain |
| 54  | BA    | 1025 | G    | Sidechain |
| 54  | BA    | 1026 | G    | Sidechain |
| 54  | BA    | 1027 | A    | Sidechain |
| 54  | BA    | 1030 | C    | Sidechain |
| 54  | BA    | 1034 | G    | Sidechain |
| 54  | BA    | 1040 | A    | Sidechain |
| 54  | BA    | 1042 | G    | Sidechain |
| 54  | BA    | 1047 | G    | Sidechain |
| 54  | BA    | 1055 | G    | Sidechain |
| 54  | BA    | 106  | C    | Sidechain |
| 54  | BA    | 1061 | U    | Sidechain |
| 54  | BA    | 1064 | C    | Sidechain |
| 54  | BA    | 1068 | G    | Sidechain |
| 54  | BA    | 1070 | A    | Sidechain |
| 54  | BA    | 1071 | G    | Sidechain |
| 54  | BA    | 1076 | C    | Sidechain |
| 54  | BA    | 1081 | U    | Sidechain |
| 54  | BA    | 1095 | A    | Sidechain |
| 54  | BA    | 1099 | G    | Sidechain |
| 54  | BA    | 11   | C    | Sidechain |
| 54  | BA    | 110  | G    | Sidechain |
| 54  | BA    | 1106 | G    | Sidechain |
| 54  | BA    | 1109 | C    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 1112 | G    | Sidechain |
| 54  | BA    | 1114 | C    | Sidechain |
| 54  | BA    | 112  | U    | Sidechain |
| 54  | BA    | 1124 | G    | Sidechain |
| 54  | BA    | 1128 | G    | Sidechain |
| 54  | BA    | 113  | U    | Sidechain |
| 54  | BA    | 1132 | U    | Sidechain |
| 54  | BA    | 1135 | C    | Sidechain |
| 54  | BA    | 1138 | G    | Sidechain |
| 54  | BA    | 1139 | G    | Sidechain |
| 54  | BA    | 1143 | A    | Sidechain |
| 54  | BA    | 1144 | A    | Sidechain |
| 54  | BA    | 1148 | U    | Sidechain |
| 54  | BA    | 1149 | G    | Sidechain |
| 54  | BA    | 1151 | A    | Sidechain |
| 54  | BA    | 1157 | G    | Sidechain |
| 54  | BA    | 1158 | C    | Sidechain |
| 54  | BA    | 1171 | G    | Sidechain |
| 54  | BA    | 1175 | A    | Sidechain |
| 54  | BA    | 1178 | C    | Sidechain |
| 54  | BA    | 1179 | G    | Sidechain |
| 54  | BA    | 1186 | G    | Sidechain |
| 54  | BA    | 1190 | G    | Sidechain |
| 54  | BA    | 1198 | U    | Sidechain |
| 54  | BA    | 1202 | G    | Sidechain |
| 54  | BA    | 121  | G    | Sidechain |
| 54  | BA    | 1210 | G    | Sidechain |
| 54  | BA    | 1212 | G    | Sidechain |
| 54  | BA    | 1216 | G    | Sidechain |
| 54  | BA    | 1220 | G    | Sidechain |
| 54  | BA    | 1223 | G    | Sidechain |
| 54  | BA    | 1224 | U    | Sidechain |
| 54  | BA    | 1236 | G    | Sidechain |
| 54  | BA    | 1237 | A    | Sidechain |
| 54  | BA    | 1239 | G    | Sidechain |
| 54  | BA    | 124  | G    | Sidechain |
| 54  | BA    | 1246 | A    | Sidechain |
| 54  | BA    | 1251 | C    | Sidechain |
| 54  | BA    | 1262 | A    | Sidechain |
| 54  | BA    | 1263 | U    | Sidechain |
| 54  | BA    | 1265 | A    | Sidechain |
| 54  | BA    | 1266 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 1270 | C    | Sidechain |
| 54  | BA    | 1273 | U    | Sidechain |
| 54  | BA    | 1283 | G    | Sidechain |
| 54  | BA    | 1287 | A    | Sidechain |
| 54  | BA    | 1289 | C    | Sidechain |
| 54  | BA    | 1290 | C    | Sidechain |
| 54  | BA    | 1293 | C    | Sidechain |
| 54  | BA    | 1307 | A    | Sidechain |
| 54  | BA    | 1309 | G    | Sidechain |
| 54  | BA    | 1313 | U    | Sidechain |
| 54  | BA    | 1315 | C    | Sidechain |
| 54  | BA    | 1316 | U    | Sidechain |
| 54  | BA    | 1318 | U    | Sidechain |
| 54  | BA    | 1319 | C    | Sidechain |
| 54  | BA    | 1320 | C    | Sidechain |
| 54  | BA    | 1323 | C    | Sidechain |
| 54  | BA    | 1331 | G    | Sidechain |
| 54  | BA    | 1338 | G    | Sidechain |
| 54  | BA    | 1340 | U    | Sidechain |
| 54  | BA    | 1350 | C    | Sidechain |
| 54  | BA    | 1352 | U    | Sidechain |
| 54  | BA    | 1355 | G    | Sidechain |
| 54  | BA    | 1360 | G    | Sidechain |
| 54  | BA    | 1361 | G    | Sidechain |
| 54  | BA    | 1369 | G    | Sidechain |
| 54  | BA    | 1370 | C    | Sidechain |
| 54  | BA    | 1376 | C    | Sidechain |
| 54  | BA    | 1378 | A    | Sidechain |
| 54  | BA    | 138  | U    | Sidechain |
| 54  | BA    | 1386 | C    | Sidechain |
| 54  | BA    | 1387 | A    | Sidechain |
| 54  | BA    | 1389 | G    | Sidechain |
| 54  | BA    | 1391 | U    | Sidechain |
| 54  | BA    | 1393 | A    | Sidechain |
| 54  | BA    | 1395 | A    | Sidechain |
| 54  | BA    | 1396 | U    | Sidechain |
| 54  | BA    | 1397 | U    | Sidechain |
| 54  | BA    | 1399 | C    | Sidechain |
| 54  | BA    | 140  | C    | Sidechain |
| 54  | BA    | 1404 | C    | Sidechain |
| 54  | BA    | 1408 | G    | Sidechain |
| 54  | BA    | 141  | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 1412 | U    | Sidechain |
| 54  | BA    | 1414 | C    | Sidechain |
| 54  | BA    | 1415 | U    | Sidechain |
| 54  | BA    | 1416 | G    | Sidechain |
| 54  | BA    | 1417 | C    | Sidechain |
| 54  | BA    | 1419 | A    | Sidechain |
| 54  | BA    | 1424 | G    | Sidechain |
| 54  | BA    | 143  | C    | Sidechain |
| 54  | BA    | 1432 | G    | Sidechain |
| 54  | BA    | 1433 | A    | Sidechain |
| 54  | BA    | 1439 | A    | Sidechain |
| 54  | BA    | 1442 | U    | Sidechain |
| 54  | BA    | 1445 | G    | Sidechain |
| 54  | BA    | 1448 | G    | Sidechain |
| 54  | BA    | 1449 | G    | Sidechain |
| 54  | BA    | 1450 | G    | Sidechain |
| 54  | BA    | 1454 | C    | Sidechain |
| 54  | BA    | 1456 | G    | Sidechain |
| 54  | BA    | 1460 | U    | Sidechain |
| 54  | BA    | 1465 | G    | Sidechain |
| 54  | BA    | 1478 | G    | Sidechain |
| 54  | BA    | 1480 | C    | Sidechain |
| 54  | BA    | 1487 | U    | Sidechain |
| 54  | BA    | 1488 | C    | Sidechain |
| 54  | BA    | 1489 | C    | Sidechain |
| 54  | BA    | 1492 | G    | Sidechain |
| 54  | BA    | 1494 | A    | Sidechain |
| 54  | BA    | 1495 | A    | Sidechain |
| 54  | BA    | 1507 | C    | Sidechain |
| 54  | BA    | 1509 | A    | Sidechain |
| 54  | BA    | 1519 | G    | Sidechain |
| 54  | BA    | 152  | A    | Sidechain |
| 54  | BA    | 1525 | A    | Sidechain |
| 54  | BA    | 153  | U    | Sidechain |
| 54  | BA    | 1530 | G    | Sidechain |
| 54  | BA    | 1535 | A    | Sidechain |
| 54  | BA    | 1536 | C    | Sidechain |
| 54  | BA    | 1538 | G    | Sidechain |
| 54  | BA    | 1539 | U    | Sidechain |
| 54  | BA    | 154  | U    | Sidechain |
| 54  | BA    | 1540 | G    | Sidechain |
| 54  | BA    | 1544 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 1546 | G    | Sidechain |
| 54  | BA    | 155  | A    | Sidechain |
| 54  | BA    | 1554 | U    | Sidechain |
| 54  | BA    | 1555 | G    | Sidechain |
| 54  | BA    | 1560 | G    | Sidechain |
| 54  | BA    | 1561 | C    | Sidechain |
| 54  | BA    | 1562 | U    | Sidechain |
| 54  | BA    | 1564 | C    | Sidechain |
| 54  | BA    | 1567 | G    | Sidechain |
| 54  | BA    | 1568 | G    | Sidechain |
| 54  | BA    | 1569 | A    | Sidechain |
| 54  | BA    | 1586 | A    | Sidechain |
| 54  | BA    | 1587 | G    | Sidechain |
| 54  | BA    | 1595 | C    | Sidechain |
| 54  | BA    | 1596 | A    | Sidechain |
| 54  | BA    | 1597 | A    | Sidechain |
| 54  | BA    | 1599 | U    | Sidechain |
| 54  | BA    | 160  | A    | Sidechain |
| 54  | BA    | 1601 | G    | Sidechain |
| 54  | BA    | 1602 | U    | Sidechain |
| 54  | BA    | 1604 | C    | Sidechain |
| 54  | BA    | 1606 | C    | Sidechain |
| 54  | BA    | 1610 | A    | Sidechain |
| 54  | BA    | 1621 | U    | Sidechain |
| 54  | BA    | 1631 | G    | Sidechain |
| 54  | BA    | 1632 | A    | Sidechain |
| 54  | BA    | 1634 | A    | Sidechain |
| 54  | BA    | 1638 | C    | Sidechain |
| 54  | BA    | 1646 | C    | Sidechain |
| 54  | BA    | 1649 | G    | Sidechain |
| 54  | BA    | 165  | A    | Sidechain |
| 54  | BA    | 1657 | U    | Sidechain |
| 54  | BA    | 1662 | U    | Sidechain |
| 54  | BA    | 1664 | A    | Sidechain |
| 54  | BA    | 1666 | G    | Sidechain |
| 54  | BA    | 1671 | U    | Sidechain |
| 54  | BA    | 1672 | A    | Sidechain |
| 54  | BA    | 1674 | G    | Sidechain |
| 54  | BA    | 1677 | A    | Sidechain |
| 54  | BA    | 1681 | G    | Sidechain |
| 54  | BA    | 1682 | G    | Sidechain |
| 54  | BA    | 1683 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 1684 | G    | Sidechain |
| 54  | BA    | 1698 | A    | Sidechain |
| 54  | BA    | 17   | G    | Sidechain |
| 54  | BA    | 1700 | A    | Sidechain |
| 54  | BA    | 1704 | C    | Sidechain |
| 54  | BA    | 1705 | A    | Sidechain |
| 54  | BA    | 1709 | U    | Sidechain |
| 54  | BA    | 1710 | G    | Sidechain |
| 54  | BA    | 1724 | G    | Sidechain |
| 54  | BA    | 1727 | C    | Sidechain |
| 54  | BA    | 1730 | C    | Sidechain |
| 54  | BA    | 1731 | G    | Sidechain |
| 54  | BA    | 1732 | C    | Sidechain |
| 54  | BA    | 1741 | C    | Sidechain |
| 54  | BA    | 1743 | G    | Sidechain |
| 54  | BA    | 1747 | U    | Sidechain |
| 54  | BA    | 1752 | C    | Sidechain |
| 54  | BA    | 1753 | G    | Sidechain |
| 54  | BA    | 1756 | G    | Sidechain |
| 54  | BA    | 1758 | U    | Sidechain |
| 54  | BA    | 1759 | A    | Sidechain |
| 54  | BA    | 1762 | A    | Sidechain |
| 54  | BA    | 177  | G    | Sidechain |
| 54  | BA    | 1773 | A    | Sidechain |
| 54  | BA    | 1774 | C    | Sidechain |
| 54  | BA    | 1788 | C    | Sidechain |
| 54  | BA    | 1790 | C    | Sidechain |
| 54  | BA    | 1797 | G    | Sidechain |
| 54  | BA    | 180  | G    | Sidechain |
| 54  | BA    | 1807 | G    | Sidechain |
| 54  | BA    | 1816 | C    | Sidechain |
| 54  | BA    | 1820 | U    | Sidechain |
| 54  | BA    | 1823 | G    | Sidechain |
| 54  | BA    | 1827 | U    | Sidechain |
| 54  | BA    | 1830 | C    | Sidechain |
| 54  | BA    | 1831 | G    | Sidechain |
| 54  | BA    | 1832 | C    | Sidechain |
| 54  | BA    | 1844 | C    | Sidechain |
| 54  | BA    | 1847 | A    | Sidechain |
| 54  | BA    | 1853 | A    | Sidechain |
| 54  | BA    | 1857 | G    | Sidechain |
| 54  | BA    | 1861 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 1866 | A    | Sidechain |
| 54  | BA    | 1867 | G    | Sidechain |
| 54  | BA    | 1871 | A    | Sidechain |
| 54  | BA    | 1874 | C    | Sidechain |
| 54  | BA    | 1876 | A    | Sidechain |
| 54  | BA    | 1884 | G    | Sidechain |
| 54  | BA    | 1888 | G    | Sidechain |
| 54  | BA    | 189  | G    | Sidechain |
| 54  | BA    | 1891 | G    | Sidechain |
| 54  | BA    | 1894 | C    | Sidechain |
| 54  | BA    | 1897 | G    | Sidechain |
| 54  | BA    | 19   | A    | Sidechain |
| 54  | BA    | 1902 | C    | Sidechain |
| 54  | BA    | 1912 | A    | Sidechain |
| 54  | BA    | 1915 | U    | Sidechain |
| 54  | BA    | 1929 | G    | Sidechain |
| 54  | BA    | 1931 | U    | Sidechain |
| 54  | BA    | 1932 | A    | Sidechain |
| 54  | BA    | 1933 | G    | Sidechain |
| 54  | BA    | 1935 | G    | Sidechain |
| 54  | BA    | 1938 | A    | Sidechain |
| 54  | BA    | 1940 | U    | Sidechain |
| 54  | BA    | 1942 | C    | Sidechain |
| 54  | BA    | 1943 | U    | Sidechain |
| 54  | BA    | 1944 | U    | Sidechain |
| 54  | BA    | 1945 | G    | Sidechain |
| 54  | BA    | 195  | A    | Sidechain |
| 54  | BA    | 1950 | G    | Sidechain |
| 54  | BA    | 196  | A    | Sidechain |
| 54  | BA    | 1960 | A    | Sidechain |
| 54  | BA    | 1961 | C    | Sidechain |
| 54  | BA    | 1962 | C    | Sidechain |
| 54  | BA    | 197  | A    | Sidechain |
| 54  | BA    | 1971 | U    | Sidechain |
| 54  | BA    | 1972 | G    | Sidechain |
| 54  | BA    | 1974 | C    | Sidechain |
| 54  | BA    | 1977 | A    | Sidechain |
| 54  | BA    | 1980 | G    | Sidechain |
| 54  | BA    | 1982 | U    | Sidechain |
| 54  | BA    | 1989 | G    | Sidechain |
| 54  | BA    | 1993 | U    | Sidechain |
| 54  | BA    | 1997 | C    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 2    | G    | Sidechain |
| 54  | BA    | 2002 | G    | Sidechain |
| 54  | BA    | 2014 | A    | Sidechain |
| 54  | BA    | 2017 | U    | Sidechain |
| 54  | BA    | 2018 | G    | Sidechain |
| 54  | BA    | 2020 | A    | Sidechain |
| 54  | BA    | 2022 | U    | Sidechain |
| 54  | BA    | 203  | A    | Sidechain |
| 54  | BA    | 2030 | A    | Sidechain |
| 54  | BA    | 2037 | A    | Sidechain |
| 54  | BA    | 2038 | G    | Sidechain |
| 54  | BA    | 2046 | G    | Sidechain |
| 54  | BA    | 205  | G    | Sidechain |
| 54  | BA    | 2056 | G    | Sidechain |
| 54  | BA    | 2059 | A    | Sidechain |
| 54  | BA    | 2064 | C    | Sidechain |
| 54  | BA    | 2067 | G    | Sidechain |
| 54  | BA    | 207  | A    | Sidechain |
| 54  | BA    | 2073 | C    | Sidechain |
| 54  | BA    | 2074 | U    | Sidechain |
| 54  | BA    | 2077 | A    | Sidechain |
| 54  | BA    | 208  | C    | Sidechain |
| 54  | BA    | 2085 | U    | Sidechain |
| 54  | BA    | 2097 | A    | Sidechain |
| 54  | BA    | 2099 | U    | Sidechain |
| 54  | BA    | 210  | C    | Sidechain |
| 54  | BA    | 2100 | G    | Sidechain |
| 54  | BA    | 2101 | A    | Sidechain |
| 54  | BA    | 2105 | U    | Sidechain |
| 54  | BA    | 2106 | U    | Sidechain |
| 54  | BA    | 2109 | U    | Sidechain |
| 54  | BA    | 2115 | G    | Sidechain |
| 54  | BA    | 2126 | A    | Sidechain |
| 54  | BA    | 2130 | U    | Sidechain |
| 54  | BA    | 2131 | U    | Sidechain |
| 54  | BA    | 2134 | A    | Sidechain |
| 54  | BA    | 2136 | G    | Sidechain |
| 54  | BA    | 2144 | G    | Sidechain |
| 54  | BA    | 2154 | A    | Sidechain |
| 54  | BA    | 2164 | C    | Sidechain |
| 54  | BA    | 2165 | C    | Sidechain |
| 54  | BA    | 2166 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 2168 | G    | Sidechain |
| 54  | BA    | 2179 | C    | Sidechain |
| 54  | BA    | 2180 | U    | Sidechain |
| 54  | BA    | 2181 | U    | Sidechain |
| 54  | BA    | 2186 | G    | Sidechain |
| 54  | BA    | 2188 | U    | Sidechain |
| 54  | BA    | 2193 | G    | Sidechain |
| 54  | BA    | 2196 | C    | Sidechain |
| 54  | BA    | 2197 | U    | Sidechain |
| 54  | BA    | 2199 | A    | Sidechain |
| 54  | BA    | 2204 | G    | Sidechain |
| 54  | BA    | 2206 | C    | Sidechain |
| 54  | BA    | 2207 | C    | Sidechain |
| 54  | BA    | 221  | A    | Sidechain |
| 54  | BA    | 2210 | U    | Sidechain |
| 54  | BA    | 2213 | U    | Sidechain |
| 54  | BA    | 2216 | G    | Sidechain |
| 54  | BA    | 2217 | G    | Sidechain |
| 54  | BA    | 2218 | G    | Sidechain |
| 54  | BA    | 2225 | A    | Sidechain |
| 54  | BA    | 2227 | A    | Sidechain |
| 54  | BA    | 2233 | U    | Sidechain |
| 54  | BA    | 2235 | G    | Sidechain |
| 54  | BA    | 2236 | U    | Sidechain |
| 54  | BA    | 2239 | G    | Sidechain |
| 54  | BA    | 2241 | A    | Sidechain |
| 54  | BA    | 2249 | U    | Sidechain |
| 54  | BA    | 2259 | U    | Sidechain |
| 54  | BA    | 2266 | A    | Sidechain |
| 54  | BA    | 2267 | A    | Sidechain |
| 54  | BA    | 2268 | A    | Sidechain |
| 54  | BA    | 2271 | G    | Sidechain |
| 54  | BA    | 2281 | A    | Sidechain |
| 54  | BA    | 2282 | G    | Sidechain |
| 54  | BA    | 2283 | C    | Sidechain |
| 54  | BA    | 2287 | A    | Sidechain |
| 54  | BA    | 2294 | G    | Sidechain |
| 54  | BA    | 2296 | U    | Sidechain |
| 54  | BA    | 2300 | C    | Sidechain |
| 54  | BA    | 2302 | U    | Sidechain |
| 54  | BA    | 2305 | U    | Sidechain |
| 54  | BA    | 2308 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 231  | A    | Sidechain |
| 54  | BA    | 2321 | U    | Sidechain |
| 54  | BA    | 2323 | G    | Sidechain |
| 54  | BA    | 2324 | U    | Sidechain |
| 54  | BA    | 2327 | A    | Sidechain |
| 54  | BA    | 2328 | A    | Sidechain |
| 54  | BA    | 2330 | G    | Sidechain |
| 54  | BA    | 2333 | A    | Sidechain |
| 54  | BA    | 2336 | A    | Sidechain |
| 54  | BA    | 2337 | G    | Sidechain |
| 54  | BA    | 2339 | C    | Sidechain |
| 54  | BA    | 2340 | A    | Sidechain |
| 54  | BA    | 2347 | C    | Sidechain |
| 54  | BA    | 235  | U    | Sidechain |
| 54  | BA    | 2352 | A    | Sidechain |
| 54  | BA    | 2357 | G    | Sidechain |
| 54  | BA    | 2362 | C    | Sidechain |
| 54  | BA    | 2367 | G    | Sidechain |
| 54  | BA    | 2369 | A    | Sidechain |
| 54  | BA    | 2375 | G    | Sidechain |
| 54  | BA    | 2381 | A    | Sidechain |
| 54  | BA    | 2385 | C    | Sidechain |
| 54  | BA    | 2389 | G    | Sidechain |
| 54  | BA    | 239  | C    | Sidechain |
| 54  | BA    | 2390 | U    | Sidechain |
| 54  | BA    | 240  | C    | Sidechain |
| 54  | BA    | 2406 | A    | Sidechain |
| 54  | BA    | 2411 | A    | Sidechain |
| 54  | BA    | 2413 | G    | Sidechain |
| 54  | BA    | 2425 | A    | Sidechain |
| 54  | BA    | 2427 | C    | Sidechain |
| 54  | BA    | 2428 | G    | Sidechain |
| 54  | BA    | 2429 | G    | Sidechain |
| 54  | BA    | 2432 | A    | Sidechain |
| 54  | BA    | 2433 | A    | Sidechain |
| 54  | BA    | 2439 | A    | Sidechain |
| 54  | BA    | 244  | A    | Sidechain |
| 54  | BA    | 2442 | C    | Sidechain |
| 54  | BA    | 2448 | A    | Sidechain |
| 54  | BA    | 2450 | A    | Sidechain |
| 54  | BA    | 2451 | A    | Sidechain |
| 54  | BA    | 2455 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 2456 | C    | Sidechain |
| 54  | BA    | 2458 | G    | Sidechain |
| 54  | BA    | 2461 | A    | Sidechain |
| 54  | BA    | 2462 | C    | Sidechain |
| 54  | BA    | 2464 | G    | Sidechain |
| 54  | BA    | 2465 | C    | Sidechain |
| 54  | BA    | 2466 | C    | Sidechain |
| 54  | BA    | 2468 | A    | Sidechain |
| 54  | BA    | 2472 | G    | Sidechain |
| 54  | BA    | 2475 | C    | Sidechain |
| 54  | BA    | 2484 | G    | Sidechain |
| 54  | BA    | 2485 | G    | Sidechain |
| 54  | BA    | 2488 | G    | Sidechain |
| 54  | BA    | 2489 | U    | Sidechain |
| 54  | BA    | 2498 | C    | Sidechain |
| 54  | BA    | 2499 | C    | Sidechain |
| 54  | BA    | 250  | G    | Sidechain |
| 54  | BA    | 2500 | U    | Sidechain |
| 54  | BA    | 2503 | A    | Sidechain |
| 54  | BA    | 2508 | G    | Sidechain |
| 54  | BA    | 2509 | G    | Sidechain |
| 54  | BA    | 2517 | C    | Sidechain |
| 54  | BA    | 2529 | G    | Sidechain |
| 54  | BA    | 2533 | U    | Sidechain |
| 54  | BA    | 2536 | G    | Sidechain |
| 54  | BA    | 2540 | C    | Sidechain |
| 54  | BA    | 2550 | G    | Sidechain |
| 54  | BA    | 2557 | G    | Sidechain |
| 54  | BA    | 2558 | C    | Sidechain |
| 54  | BA    | 2564 | A    | Sidechain |
| 54  | BA    | 2566 | A    | Sidechain |
| 54  | BA    | 2567 | G    | Sidechain |
| 54  | BA    | 2571 | U    | Sidechain |
| 54  | BA    | 2573 | C    | Sidechain |
| 54  | BA    | 2576 | G    | Sidechain |
| 54  | BA    | 2578 | G    | Sidechain |
| 54  | BA    | 2581 | G    | Sidechain |
| 54  | BA    | 2589 | A    | Sidechain |
| 54  | BA    | 2590 | A    | Sidechain |
| 54  | BA    | 2592 | G    | Sidechain |
| 54  | BA    | 2595 | G    | Sidechain |
| 54  | BA    | 2601 | C    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 2607 | G    | Sidechain |
| 54  | BA    | 2608 | G    | Sidechain |
| 54  | BA    | 2612 | C    | Sidechain |
| 54  | BA    | 2613 | U    | Sidechain |
| 54  | BA    | 2617 | U    | Sidechain |
| 54  | BA    | 2625 | G    | Sidechain |
| 54  | BA    | 2626 | C    | Sidechain |
| 54  | BA    | 2630 | G    | Sidechain |
| 54  | BA    | 2631 | G    | Sidechain |
| 54  | BA    | 2633 | G    | Sidechain |
| 54  | BA    | 2637 | U    | Sidechain |
| 54  | BA    | 2638 | G    | Sidechain |
| 54  | BA    | 2640 | G    | Sidechain |
| 54  | BA    | 2641 | G    | Sidechain |
| 54  | BA    | 2643 | G    | Sidechain |
| 54  | BA    | 2649 | C    | Sidechain |
| 54  | BA    | 265  | A    | Sidechain |
| 54  | BA    | 2655 | G    | Sidechain |
| 54  | BA    | 2656 | U    | Sidechain |
| 54  | BA    | 2657 | A    | Sidechain |
| 54  | BA    | 2661 | G    | Sidechain |
| 54  | BA    | 2663 | G    | Sidechain |
| 54  | BA    | 2665 | A    | Sidechain |
| 54  | BA    | 2666 | C    | Sidechain |
| 54  | BA    | 2674 | G    | Sidechain |
| 54  | BA    | 2675 | A    | Sidechain |
| 54  | BA    | 2681 | C    | Sidechain |
| 54  | BA    | 2682 | A    | Sidechain |
| 54  | BA    | 2689 | U    | Sidechain |
| 54  | BA    | 2690 | U    | Sidechain |
| 54  | BA    | 2698 | U    | Sidechain |
| 54  | BA    | 27   | G    | Sidechain |
| 54  | BA    | 2704 | C    | Sidechain |
| 54  | BA    | 2706 | A    | Sidechain |
| 54  | BA    | 271  | G    | Sidechain |
| 54  | BA    | 2718 | G    | Sidechain |
| 54  | BA    | 272  | A    | Sidechain |
| 54  | BA    | 2721 | A    | Sidechain |
| 54  | BA    | 2726 | A    | Sidechain |
| 54  | BA    | 2729 | G    | Sidechain |
| 54  | BA    | 2731 | G    | Sidechain |
| 54  | BA    | 2732 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | BA    | 2738 | A    | Sidechain |
| 54  | BA    | 2740 | A    | Sidechain |
| 54  | BA    | 2745 | C    | Sidechain |
| 54  | BA    | 2756 | U    | Sidechain |
| 54  | BA    | 2760 | C    | Sidechain |
| 54  | BA    | 2762 | C    | Sidechain |
| 54  | BA    | 2765 | A    | Sidechain |
| 54  | BA    | 2777 | G    | Sidechain |
| 54  | BA    | 2780 | G    | Sidechain |
| 54  | BA    | 2784 | U    | Sidechain |
| 54  | BA    | 279  | A    | Sidechain |
| 54  | BA    | 2790 | U    | Sidechain |
| 54  | BA    | 2793 | C    | Sidechain |
| 54  | BA    | 2794 | C    | Sidechain |
| 54  | BA    | 2798 | U    | Sidechain |
| 54  | BA    | 2808 | G    | Sidechain |
| 54  | BA    | 281  | C    | Sidechain |
| 54  | BA    | 2810 | A    | Sidechain |
| 54  | BA    | 2811 | G    | Sidechain |
| 54  | BA    | 2816 | G    | Sidechain |
| 54  | BA    | 2819 | G    | Sidechain |
| 54  | BA    | 2824 | C    | Sidechain |
| 54  | BA    | 2831 | G    | Sidechain |
| 54  | BA    | 2832 | U    | Sidechain |
| 54  | BA    | 2833 | U    | Sidechain |
| 54  | BA    | 2835 | A    | Sidechain |
| 54  | BA    | 2836 | U    | Sidechain |
| 54  | BA    | 2852 | G    | Sidechain |
| 54  | BA    | 2856 | A    | Sidechain |
| 54  | BA    | 2859 | G    | Sidechain |
| 54  | BA    | 2862 | G    | Sidechain |
| 54  | BA    | 2864 | G    | Sidechain |
| 54  | BA    | 2868 | A    | Sidechain |
| 54  | BA    | 2876 | G    | Sidechain |
| 54  | BA    | 2877 | G    | Sidechain |
| 54  | BA    | 2886 | A    | Sidechain |
| 54  | BA    | 2889 | C    | Sidechain |
| 54  | BA    | 2896 | C    | Sidechain |
| 54  | BA    | 2899 | A    | Sidechain |
| 54  | BA    | 2901 | C    | Sidechain |
| 54  | BA    | 2902 | C    | Sidechain |
| 54  | BA    | 291  | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 54  | BA    | 295 | G    | Sidechain |
| 54  | BA    | 299 | A    | Sidechain |
| 54  | BA    | 303 | G    | Sidechain |
| 54  | BA    | 307 | G    | Sidechain |
| 54  | BA    | 308 | G    | Sidechain |
| 54  | BA    | 31  | C    | Sidechain |
| 54  | BA    | 313 | G    | Sidechain |
| 54  | BA    | 317 | G    | Sidechain |
| 54  | BA    | 326 | G    | Sidechain |
| 54  | BA    | 33  | C    | Sidechain |
| 54  | BA    | 333 | G    | Sidechain |
| 54  | BA    | 334 | C    | Sidechain |
| 54  | BA    | 336 | C    | Sidechain |
| 54  | BA    | 337 | C    | Sidechain |
| 54  | BA    | 347 | A    | Sidechain |
| 54  | BA    | 354 | A    | Sidechain |
| 54  | BA    | 361 | G    | Sidechain |
| 54  | BA    | 362 | A    | Sidechain |
| 54  | BA    | 363 | G    | Sidechain |
| 54  | BA    | 369 | U    | Sidechain |
| 54  | BA    | 370 | G    | Sidechain |
| 54  | BA    | 378 | C    | Sidechain |
| 54  | BA    | 389 | G    | Sidechain |
| 54  | BA    | 392 | U    | Sidechain |
| 54  | BA    | 394 | C    | Sidechain |
| 54  | BA    | 395 | U    | Sidechain |
| 54  | BA    | 410 | G    | Sidechain |
| 54  | BA    | 418 | C    | Sidechain |
| 54  | BA    | 419 | U    | Sidechain |
| 54  | BA    | 422 | A    | Sidechain |
| 54  | BA    | 426 | C    | Sidechain |
| 54  | BA    | 428 | A    | Sidechain |
| 54  | BA    | 43  | G    | Sidechain |
| 54  | BA    | 431 | U    | Sidechain |
| 54  | BA    | 433 | C    | Sidechain |
| 54  | BA    | 436 | C    | Sidechain |
| 54  | BA    | 440 | C    | Sidechain |
| 54  | BA    | 446 | G    | Sidechain |
| 54  | BA    | 449 | A    | Sidechain |
| 54  | BA    | 450 | G    | Sidechain |
| 54  | BA    | 454 | A    | Sidechain |
| 54  | BA    | 456 | C    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 54  | BA    | 458 | G    | Sidechain |
| 54  | BA    | 459 | U    | Sidechain |
| 54  | BA    | 463 | G    | Sidechain |
| 54  | BA    | 47  | C    | Sidechain |
| 54  | BA    | 472 | A    | Sidechain |
| 54  | BA    | 474 | G    | Sidechain |
| 54  | BA    | 475 | C    | Sidechain |
| 54  | BA    | 476 | G    | Sidechain |
| 54  | BA    | 48  | G    | Sidechain |
| 54  | BA    | 480 | A    | Sidechain |
| 54  | BA    | 481 | G    | Sidechain |
| 54  | BA    | 488 | G    | Sidechain |
| 54  | BA    | 49  | A    | Sidechain |
| 54  | BA    | 492 | A    | Sidechain |
| 54  | BA    | 500 | G    | Sidechain |
| 54  | BA    | 501 | A    | Sidechain |
| 54  | BA    | 502 | A    | Sidechain |
| 54  | BA    | 504 | A    | Sidechain |
| 54  | BA    | 505 | A    | Sidechain |
| 54  | BA    | 507 | A    | Sidechain |
| 54  | BA    | 508 | A    | Sidechain |
| 54  | BA    | 51  | G    | Sidechain |
| 54  | BA    | 511 | U    | Sidechain |
| 54  | BA    | 514 | A    | Sidechain |
| 54  | BA    | 525 | U    | Sidechain |
| 54  | BA    | 528 | A    | Sidechain |
| 54  | BA    | 530 | G    | Sidechain |
| 54  | BA    | 533 | G    | Sidechain |
| 54  | BA    | 537 | G    | Sidechain |
| 54  | BA    | 54  | G    | Sidechain |
| 54  | BA    | 541 | A    | Sidechain |
| 54  | BA    | 548 | G    | Sidechain |
| 54  | BA    | 551 | G    | Sidechain |
| 54  | BA    | 558 | U    | Sidechain |
| 54  | BA    | 568 | U    | Sidechain |
| 54  | BA    | 577 | G    | Sidechain |
| 54  | BA    | 586 | A    | Sidechain |
| 54  | BA    | 588 | U    | Sidechain |
| 54  | BA    | 589 | U    | Sidechain |
| 54  | BA    | 595 | C    | Sidechain |
| 54  | BA    | 599 | A    | Sidechain |
| 54  | BA    | 60  | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 54  | BA    | 600 | G    | Sidechain |
| 54  | BA    | 605 | G    | Sidechain |
| 54  | BA    | 608 | A    | Sidechain |
| 54  | BA    | 611 | C    | Sidechain |
| 54  | BA    | 614 | A    | Sidechain |
| 54  | BA    | 621 | A    | Sidechain |
| 54  | BA    | 626 | A    | Sidechain |
| 54  | BA    | 628 | G    | Sidechain |
| 54  | BA    | 629 | G    | Sidechain |
| 54  | BA    | 630 | G    | Sidechain |
| 54  | BA    | 631 | A    | Sidechain |
| 54  | BA    | 638 | G    | Sidechain |
| 54  | BA    | 64  | A    | Sidechain |
| 54  | BA    | 641 | U    | Sidechain |
| 54  | BA    | 646 | U    | Sidechain |
| 54  | BA    | 65  | U    | Sidechain |
| 54  | BA    | 661 | A    | Sidechain |
| 54  | BA    | 662 | G    | Sidechain |
| 54  | BA    | 663 | G    | Sidechain |
| 54  | BA    | 665 | U    | Sidechain |
| 54  | BA    | 670 | A    | Sidechain |
| 54  | BA    | 671 | C    | Sidechain |
| 54  | BA    | 674 | G    | Sidechain |
| 54  | BA    | 676 | A    | Sidechain |
| 54  | BA    | 68  | G    | Sidechain |
| 54  | BA    | 686 | U    | Sidechain |
| 54  | BA    | 69  | C    | Sidechain |
| 54  | BA    | 697 | G    | Sidechain |
| 54  | BA    | 707 | G    | Sidechain |
| 54  | BA    | 71  | A    | Sidechain |
| 54  | BA    | 714 | U    | Sidechain |
| 54  | BA    | 718 | A    | Sidechain |
| 54  | BA    | 724 | U    | Sidechain |
| 54  | BA    | 725 | G    | Sidechain |
| 54  | BA    | 728 | G    | Sidechain |
| 54  | BA    | 730 | A    | Sidechain |
| 54  | BA    | 738 | G    | Sidechain |
| 54  | BA    | 74  | A    | Sidechain |
| 54  | BA    | 746 | U    | Sidechain |
| 54  | BA    | 75  | G    | Sidechain |
| 54  | BA    | 750 | A    | Sidechain |
| 54  | BA    | 754 | U    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 54  | BA    | 76  | C    | Sidechain |
| 54  | BA    | 771 | G    | Sidechain |
| 54  | BA    | 773 | U    | Sidechain |
| 54  | BA    | 775 | G    | Sidechain |
| 54  | BA    | 782 | A    | Sidechain |
| 54  | BA    | 79  | C    | Sidechain |
| 54  | BA    | 799 | G    | Sidechain |
| 54  | BA    | 800 | A    | Sidechain |
| 54  | BA    | 801 | G    | Sidechain |
| 54  | BA    | 802 | A    | Sidechain |
| 54  | BA    | 803 | U    | Sidechain |
| 54  | BA    | 804 | A    | Sidechain |
| 54  | BA    | 810 | U    | Sidechain |
| 54  | BA    | 811 | U    | Sidechain |
| 54  | BA    | 816 | C    | Sidechain |
| 54  | BA    | 822 | G    | Sidechain |
| 54  | BA    | 823 | C    | Sidechain |
| 54  | BA    | 827 | U    | Sidechain |
| 54  | BA    | 828 | U    | Sidechain |
| 54  | BA    | 831 | G    | Sidechain |
| 54  | BA    | 832 | U    | Sidechain |
| 54  | BA    | 837 | C    | Sidechain |
| 54  | BA    | 848 | C    | Sidechain |
| 54  | BA    | 849 | A    | Sidechain |
| 54  | BA    | 851 | C    | Sidechain |
| 54  | BA    | 853 | C    | Sidechain |
| 54  | BA    | 858 | G    | Sidechain |
| 54  | BA    | 862 | G    | Sidechain |
| 54  | BA    | 864 | G    | Sidechain |
| 54  | BA    | 869 | G    | Sidechain |
| 54  | BA    | 87  | U    | Sidechain |
| 54  | BA    | 874 | G    | Sidechain |
| 54  | BA    | 880 | G    | Sidechain |
| 54  | BA    | 886 | A    | Sidechain |
| 54  | BA    | 887 | U    | Sidechain |
| 54  | BA    | 889 | C    | Sidechain |
| 54  | BA    | 902 | C    | Sidechain |
| 54  | BA    | 906 | U    | Sidechain |
| 54  | BA    | 910 | A    | Sidechain |
| 54  | BA    | 912 | C    | Sidechain |
| 54  | BA    | 914 | G    | Sidechain |
| 54  | BA    | 928 | A    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 54  | BA    | 934 | U    | Sidechain |
| 54  | BA    | 937 | C    | Sidechain |
| 54  | BA    | 938 | G    | Sidechain |
| 54  | BA    | 94  | A    | Sidechain |
| 54  | BA    | 942 | G    | Sidechain |
| 54  | BA    | 946 | C    | Sidechain |
| 54  | BA    | 947 | A    | Sidechain |
| 54  | BA    | 950 | G    | Sidechain |
| 54  | BA    | 951 | C    | Sidechain |
| 54  | BA    | 952 | G    | Sidechain |
| 54  | BA    | 954 | G    | Sidechain |
| 54  | BA    | 955 | U    | Sidechain |
| 54  | BA    | 957 | C    | Sidechain |
| 54  | BA    | 959 | A    | Sidechain |
| 54  | BA    | 96  | C    | Sidechain |
| 54  | BA    | 966 | G    | Sidechain |
| 54  | BA    | 968 | C    | Sidechain |
| 54  | BA    | 969 | G    | Sidechain |
| 54  | BA    | 975 | A    | Sidechain |
| 54  | BA    | 976 | G    | Sidechain |
| 54  | BA    | 980 | A    | Sidechain |
| 54  | BA    | 981 | A    | Sidechain |
| 54  | BA    | 982 | C    | Sidechain |
| 54  | BA    | 984 | A    | Sidechain |
| 54  | BA    | 986 | C    | Sidechain |
| 54  | BA    | 989 | G    | Sidechain |
| 54  | BA    | 99  | U    | Sidechain |
| 54  | BA    | 992 | C    | Sidechain |
| 54  | BA    | 993 | G    | Sidechain |
| 55  | BB    | 100 | G    | Sidechain |
| 55  | BB    | 108 | A    | Sidechain |
| 55  | BB    | 109 | A    | Sidechain |
| 55  | BB    | 11  | C    | Sidechain |
| 55  | BB    | 12  | C    | Sidechain |
| 55  | BB    | 14  | U    | Sidechain |
| 55  | BB    | 18  | G    | Sidechain |
| 55  | BB    | 27  | C    | Sidechain |
| 55  | BB    | 33  | G    | Sidechain |
| 55  | BB    | 34  | A    | Sidechain |
| 55  | BB    | 40  | U    | Sidechain |
| 55  | BB    | 41  | G    | Sidechain |
| 55  | BB    | 60  | C    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 55  | BB    | 62  | C    | Sidechain |
| 55  | BB    | 65  | U    | Sidechain |
| 55  | BB    | 69  | G    | Sidechain |
| 55  | BB    | 73  | A    | Sidechain |
| 55  | BB    | 75  | G    | Sidechain |
| 55  | BB    | 83  | G    | Sidechain |
| 55  | BB    | 93  | C    | Sidechain |
| 27  | BE    | 101 | TYR  | Sidechain |
| 37  | BO    | 7   | ARG  | Sidechain |
| 39  | BQ    | 44  | TYR  | Sidechain |
| 45  | BW    | 54  | ARG  | Sidechain |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AB    | 1708  | 0        | 1736     | 0       | 0            |
| 2   | AC    | 1625  | 0        | 1699     | 0       | 0            |
| 3   | AD    | 1643  | 0        | 1710     | 0       | 0            |
| 4   | AE    | 1109  | 0        | 1152     | 0       | 0            |
| 5   | AF    | 818   | 0        | 808      | 0       | 0            |
| 6   | AG    | 1178  | 0        | 1234     | 0       | 0            |
| 7   | AH    | 979   | 0        | 1034     | 0       | 0            |
| 8   | AI    | 1025  | 0        | 1074     | 0       | 0            |
| 9   | AJ    | 790   | 0        | 832      | 0       | 0            |
| 10  | AK    | 880   | 0        | 891      | 1       | 0            |
| 11  | AL    | 955   | 0        | 1019     | 1       | 0            |
| 12  | AM    | 877   | 0        | 937      | 0       | 0            |
| 13  | AN    | 805   | 0        | 844      | 0       | 0            |
| 14  | AO    | 714   | 0        | 737      | 0       | 0            |
| 15  | AP    | 639   | 0        | 656      | 0       | 0            |
| 16  | AQ    | 652   | 0        | 695      | 0       | 0            |
| 17  | AR    | 459   | 0        | 482      | 0       | 0            |
| 18  | AS    | 641   | 0        | 669      | 1       | 0            |
| 19  | AT    | 668   | 0        | 718      | 2       | 0            |
| 20  | AU    | 429   | 0        | 453      | 0       | 0            |
| 21  | AA    | 32828 | 0        | 16522    | 3       | 0            |
| 22  | A1    | 1627  | 0        | 832      | 1       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 23  | A2    | 309    | 0        | 158      | 0       | 0            |
| 24  | A3    | 1642   | 0        | 843      | 0       | 0            |
| 25  | BC    | 2083   | 0        | 2157     | 0       | 0            |
| 26  | BD    | 1565   | 0        | 1616     | 0       | 0            |
| 27  | BE    | 1552   | 0        | 1619     | 0       | 0            |
| 28  | BF    | 1420   | 0        | 1460     | 0       | 0            |
| 29  | BG    | 1323   | 0        | 1374     | 0       | 0            |
| 30  | BH    | 1111   | 0        | 1148     | 0       | 0            |
| 31  | BI    | 1032   | 0        | 1088     | 0       | 0            |
| 32  | BJ    | 1129   | 0        | 1162     | 0       | 0            |
| 33  | BK    | 939    | 0        | 1012     | 0       | 0            |
| 34  | BL    | 1045   | 0        | 1117     | 0       | 0            |
| 35  | BM    | 1074   | 0        | 1157     | 1       | 0            |
| 36  | BN    | 961    | 0        | 1000     | 0       | 0            |
| 37  | BO    | 892    | 0        | 923      | 0       | 0            |
| 38  | BP    | 917    | 0        | 965      | 0       | 0            |
| 39  | BQ    | 947    | 0        | 1022     | 1       | 0            |
| 40  | BR    | 816    | 0        | 839      | 0       | 0            |
| 41  | BS    | 857    | 0        | 922      | 0       | 0            |
| 42  | BT    | 739    | 0        | 807      | 0       | 0            |
| 43  | BU    | 780    | 0        | 834      | 0       | 0            |
| 44  | BV    | 753    | 0        | 780      | 0       | 0            |
| 45  | BW    | 599    | 0        | 614      | 0       | 0            |
| 46  | BX    | 625    | 0        | 655      | 0       | 0            |
| 47  | BY    | 509    | 0        | 543      | 0       | 0            |
| 48  | BZ    | 449    | 0        | 491      | 0       | 0            |
| 49  | B0    | 444    | 0        | 461      | 0       | 0            |
| 50  | B1    | 413    | 0        | 444      | 0       | 0            |
| 51  | B2    | 377    | 0        | 418      | 0       | 0            |
| 52  | B3    | 504    | 0        | 574      | 0       | 0            |
| 53  | B4    | 302    | 0        | 343      | 1       | 0            |
| 54  | BA    | 62317  | 0        | 31343    | 6       | 0            |
| 55  | BB    | 2504   | 0        | 1271     | 0       | 0            |
| 56  | B5    | 1658   | 0        | 1751     | 0       | 0            |
| 57  | A1    | 7      | 0        | 8        | 0       | 0            |
| 58  | A1    | 10     | 0        | 10       | 0       | 0            |
| All | All   | 147653 | 0        | 99663    | 16      | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:AT:40:ALA:HB1  | 19:AT:41:GLY:HA2   | 1.86                     | 0.57              |
| 54:BA:1977:A:H2'  | 54:BA:1978:A:C8    | 2.51                     | 0.46              |
| 54:BA:1709:U:H2'  | 54:BA:1710:G:C8    | 2.52                     | 0.44              |
| 18:AS:78:THR:HB   | 18:AS:79:TYR:HA    | 1.99                     | 0.44              |
| 39:BQ:40:LYS:HE2  | 39:BQ:44:TYR:CZ    | 2.53                     | 0.44              |
| 53:B4:1:MET:HA    | 53:B4:34:LYS:O     | 2.17                     | 0.44              |
| 21:AA:1412:C:H2'  | 21:AA:1413:A:C8    | 2.53                     | 0.43              |
| 10:AK:34:THR:HG21 | 21:AA:707:U:H1'    | 1.99                     | 0.43              |
| 54:BA:2318:G:H2'  | 54:BA:2319:G:C8    | 2.54                     | 0.43              |
| 54:BA:889:C:H1'   | 54:BA:890:C:C6     | 2.54                     | 0.43              |
| 19:AT:40:ALA:HB1  | 19:AT:41:GLY:CA    | 2.49                     | 0.42              |
| 54:BA:1752:C:H2'  | 54:BA:1753:G:C8    | 2.56                     | 0.41              |
| 22:A1:55:PSU:HO2' | 22:A1:57:G:H8      | 1.65                     | 0.41              |
| 54:BA:152:A:H2'   | 54:BA:153:U:C6     | 2.56                     | 0.41              |
| 35:BM:119:LEU:H   | 35:BM:119:LEU:HD23 | 1.86                     | 0.40              |
| 11:AL:47:ALA:HB3  | 21:AA:529:G:H22    | 1.87                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | AB    | 218/220 (99%) | 201 (92%) | 14 (6%)  | 3 (1%)   | 9           | 40 |
| 2   | AC    | 205/208 (99%) | 189 (92%) | 13 (6%)  | 3 (2%)   | 8           | 40 |
| 3   | AD    | 203/206 (98%) | 188 (93%) | 13 (6%)  | 2 (1%)   | 12          | 49 |
| 4   | AE    | 150/152 (99%) | 135 (90%) | 10 (7%)  | 5 (3%)   | 3           | 21 |
| 5   | AF    | 99/101 (98%)  | 81 (82%)  | 14 (14%) | 4 (4%)   | 2           | 18 |
| 6   | AG    | 150/152 (99%) | 134 (89%) | 13 (9%)  | 3 (2%)   | 6           | 31 |
| 7   | AH    | 127/130 (98%) | 117 (92%) | 5 (4%)   | 5 (4%)   | 2           | 19 |
| 8   | AI    | 126/128 (98%) | 106 (84%) | 16 (13%) | 4 (3%)   | 3           | 21 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 9   | AJ    | 98/100 (98%)  | 91 (93%)  | 2 (2%)   | 5 (5%)   | 1           | 15  |
| 10  | AK    | 116/118 (98%) | 109 (94%) | 4 (3%)   | 3 (3%)   | 4           | 25  |
| 11  | AL    | 121/124 (98%) | 109 (90%) | 9 (7%)   | 3 (2%)   | 4           | 26  |
| 12  | AM    | 112/115 (97%) | 93 (83%)  | 14 (12%) | 5 (4%)   | 2           | 17  |
| 13  | AN    | 98/101 (97%)  | 88 (90%)  | 9 (9%)   | 1 (1%)   | 12          | 49  |
| 14  | AO    | 86/89 (97%)   | 80 (93%)  | 5 (6%)   | 1 (1%)   | 10          | 44  |
| 15  | AP    | 79/81 (98%)   | 71 (90%)  | 6 (8%)   | 2 (2%)   | 4           | 26  |
| 16  | AQ    | 80/82 (98%)   | 74 (92%)  | 6 (8%)   | 0        | 100         | 100 |
| 17  | AR    | 55/57 (96%)   | 50 (91%)  | 4 (7%)   | 1 (2%)   | 6           | 34  |
| 18  | AS    | 79/81 (98%)   | 69 (87%)  | 9 (11%)  | 1 (1%)   | 9           | 42  |
| 19  | AT    | 84/86 (98%)   | 73 (87%)  | 9 (11%)  | 2 (2%)   | 4           | 27  |
| 20  | AU    | 51/53 (96%)   | 32 (63%)  | 15 (29%) | 4 (8%)   | 1           | 10  |
| 25  | BC    | 270/273 (99%) | 236 (87%) | 26 (10%) | 8 (3%)   | 3           | 23  |
| 26  | BD    | 207/209 (99%) | 178 (86%) | 15 (7%)  | 14 (7%)  | 1           | 11  |
| 27  | BE    | 199/201 (99%) | 187 (94%) | 7 (4%)   | 5 (2%)   | 4           | 26  |
| 28  | BF    | 176/179 (98%) | 153 (87%) | 18 (10%) | 5 (3%)   | 4           | 24  |
| 29  | BG    | 174/177 (98%) | 160 (92%) | 11 (6%)  | 3 (2%)   | 7           | 36  |
| 30  | BH    | 147/149 (99%) | 136 (92%) | 9 (6%)   | 2 (1%)   | 9           | 40  |
| 31  | BI    | 139/142 (98%) | 127 (91%) | 11 (8%)  | 1 (1%)   | 18          | 56  |
| 32  | BJ    | 140/142 (99%) | 131 (94%) | 7 (5%)   | 2 (1%)   | 9           | 40  |
| 33  | BK    | 121/123 (98%) | 107 (88%) | 10 (8%)  | 4 (3%)   | 3           | 21  |
| 34  | BL    | 141/144 (98%) | 122 (86%) | 15 (11%) | 4 (3%)   | 4           | 24  |
| 35  | BM    | 134/136 (98%) | 121 (90%) | 8 (6%)   | 5 (4%)   | 2           | 20  |
| 36  | BN    | 119/121 (98%) | 107 (90%) | 10 (8%)  | 2 (2%)   | 7           | 36  |
| 37  | BO    | 114/117 (97%) | 105 (92%) | 8 (7%)   | 1 (1%)   | 14          | 51  |
| 38  | BP    | 112/115 (97%) | 94 (84%)  | 11 (10%) | 7 (6%)   | 1           | 13  |
| 39  | BQ    | 115/118 (98%) | 106 (92%) | 6 (5%)   | 3 (3%)   | 4           | 25  |
| 40  | BR    | 101/103 (98%) | 92 (91%)  | 7 (7%)   | 2 (2%)   | 6           | 31  |
| 41  | BS    | 108/110 (98%) | 100 (93%) | 5 (5%)   | 3 (3%)   | 4           | 24  |
| 42  | BT    | 92/94 (98%)   | 77 (84%)  | 8 (9%)   | 7 (8%)   | 1           | 10  |
| 43  | BU    | 101/104 (97%) | 85 (84%)  | 10 (10%) | 6 (6%)   | 1           | 13  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 44  | BV    | 92/94 (98%)     | 86 (94%)   | 3 (3%)   | 3 (3%)   | 3           | 21  |
| 45  | BW    | 78/80 (98%)     | 56 (72%)   | 16 (20%) | 6 (8%)   | 1           | 10  |
| 46  | BX    | 75/79 (95%)     | 66 (88%)   | 7 (9%)   | 2 (3%)   | 4           | 25  |
| 47  | BY    | 61/63 (97%)     | 54 (88%)   | 5 (8%)   | 2 (3%)   | 3           | 21  |
| 48  | BZ    | 56/59 (95%)     | 50 (89%)   | 5 (9%)   | 1 (2%)   | 6           | 34  |
| 49  | B0    | 54/57 (95%)     | 44 (82%)   | 9 (17%)  | 1 (2%)   | 6           | 32  |
| 50  | B1    | 50/52 (96%)     | 47 (94%)   | 3 (6%)   | 0        | 100         | 100 |
| 51  | B2    | 44/46 (96%)     | 42 (96%)   | 0        | 2 (4%)   | 2           | 17  |
| 52  | B3    | 62/65 (95%)     | 57 (92%)   | 4 (6%)   | 1 (2%)   | 7           | 38  |
| 53  | B4    | 36/38 (95%)     | 32 (89%)   | 4 (11%)  | 0        | 100         | 100 |
| 56  | B5    | 221/234 (94%)   | 206 (93%)  | 13 (6%)  | 2 (1%)   | 14          | 51  |
| All | All   | 5876/6008 (98%) | 5254 (89%) | 461 (8%) | 161 (3%) | 6           | 25  |

All (161) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AB    | 10  | LYS  |
| 5   | AF    | 90  | MET  |
| 6   | AG    | 5   | VAL  |
| 7   | AH    | 77  | VAL  |
| 10  | AK    | 125 | LYS  |
| 11  | AL    | 43  | LYS  |
| 12  | AM    | 85  | TYR  |
| 26  | BD    | 80  | TRP  |
| 26  | BD    | 170 | VAL  |
| 27  | BE    | 79  | ARG  |
| 33  | BK    | 103 | VAL  |
| 43  | BU    | 85  | ARG  |
| 46  | BX    | 43  | LYS  |
| 1   | AB    | 18  | GLN  |
| 3   | AD    | 29  | THR  |
| 4   | AE    | 105 | ILE  |
| 5   | AF    | 6   | ILE  |
| 5   | AF    | 10  | VAL  |
| 6   | AG    | 6   | ILE  |
| 9   | AJ    | 75  | ASP  |
| 9   | AJ    | 102 | LEU  |
| 12  | AM    | 3   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | AM    | 42  | VAL  |
| 12  | AM    | 104 | ASN  |
| 17  | AR    | 20  | ILE  |
| 18  | AS    | 5   | LYS  |
| 20  | AU    | 23  | GLU  |
| 25  | BC    | 189 | ALA  |
| 26  | BD    | 34  | VAL  |
| 26  | BD    | 41  | ALA  |
| 26  | BD    | 77  | ARG  |
| 26  | BD    | 119 | ALA  |
| 26  | BD    | 155 | VAL  |
| 27  | BE    | 90  | GLN  |
| 27  | BE    | 97  | ASN  |
| 27  | BE    | 147 | LEU  |
| 28  | BF    | 12  | VAL  |
| 28  | BF    | 103 | ILE  |
| 29  | BG    | 152 | ARG  |
| 33  | BK    | 25  | LEU  |
| 34  | BL    | 101 | ILE  |
| 35  | BM    | 70  | ASP  |
| 36  | BN    | 47  | VAL  |
| 37  | BO    | 89  | ASP  |
| 39  | BQ    | 87  | VAL  |
| 39  | BQ    | 91  | ARG  |
| 40  | BR    | 91  | GLN  |
| 41  | BS    | 88  | ARG  |
| 42  | BT    | 66  | LYS  |
| 42  | BT    | 68  | LYS  |
| 42  | BT    | 88  | LYS  |
| 43  | BU    | 45  | GLN  |
| 45  | BW    | 10  | ARG  |
| 47  | BY    | 23  | ARG  |
| 48  | BZ    | 32  | GLY  |
| 51  | B2    | 3   | ARG  |
| 4   | AE    | 54  | GLU  |
| 6   | AG    | 113 | LYS  |
| 8   | AI    | 127 | SER  |
| 10  | AK    | 126 | ARG  |
| 11  | AL    | 46  | SER  |
| 13  | AN    | 63  | ARG  |
| 14  | AO    | 43  | ALA  |
| 15  | AP    | 43  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | AT    | 3   | ILE  |
| 19  | AT    | 65  | LEU  |
| 25  | BC    | 43  | ASN  |
| 25  | BC    | 141 | HIS  |
| 25  | BC    | 142 | ASN  |
| 25  | BC    | 153 | LEU  |
| 26  | BD    | 40  | LEU  |
| 26  | BD    | 73  | VAL  |
| 26  | BD    | 150 | GLN  |
| 28  | BF    | 136 | ILE  |
| 30  | BH    | 148 | ALA  |
| 32  | BJ    | 81  | ILE  |
| 34  | BL    | 13  | LYS  |
| 34  | BL    | 82  | LEU  |
| 35  | BM    | 69  | PRO  |
| 35  | BM    | 110 | GLU  |
| 38  | BP    | 58  | PHE  |
| 38  | BP    | 113 | LEU  |
| 42  | BT    | 11  | LEU  |
| 43  | BU    | 5   | ARG  |
| 43  | BU    | 12  | VAL  |
| 43  | BU    | 43  | LYS  |
| 45  | BW    | 38  | ARG  |
| 45  | BW    | 44  | PHE  |
| 52  | B3    | 3   | ILE  |
| 56  | B5    | 91  | GLY  |
| 56  | B5    | 219 | GLY  |
| 2   | AC    | 195 | ILE  |
| 7   | AH    | 69  | ALA  |
| 7   | AH    | 78  | SER  |
| 8   | AI    | 120 | ALA  |
| 9   | AJ    | 45  | ARG  |
| 9   | AJ    | 57  | VAL  |
| 9   | AJ    | 92  | LEU  |
| 10  | AK    | 16  | SER  |
| 20  | AU    | 17  | ARG  |
| 20  | AU    | 49  | ALA  |
| 25  | BC    | 70  | LYS  |
| 25  | BC    | 204 | LEU  |
| 26  | BD    | 15  | PHE  |
| 26  | BD    | 51  | THR  |
| 28  | BF    | 132 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | BF    | 156 | THR  |
| 29  | BG    | 4   | ALA  |
| 29  | BG    | 22  | VAL  |
| 30  | BH    | 48  | GLU  |
| 33  | BK    | 92  | GLU  |
| 36  | BN    | 2   | ARG  |
| 38  | BP    | 74  | GLN  |
| 41  | BS    | 28  | LYS  |
| 43  | BU    | 70  | ALA  |
| 44  | BV    | 23  | ALA  |
| 44  | BV    | 24  | ASN  |
| 45  | BW    | 23  | LYS  |
| 45  | BW    | 56  | HIS  |
| 46  | BX    | 21  | LEU  |
| 47  | BY    | 7   | ARG  |
| 51  | B2    | 4   | THR  |
| 1   | AB    | 87  | ASP  |
| 2   | AC    | 189 | HIS  |
| 5   | AF    | 63  | ASN  |
| 7   | AH    | 2   | MET  |
| 8   | AI    | 55  | ASP  |
| 8   | AI    | 112 | ARG  |
| 11  | AL    | 117 | GLY  |
| 12  | AM    | 65  | GLU  |
| 15  | AP    | 17  | TYR  |
| 31  | BI    | 64  | ARG  |
| 32  | BJ    | 25  | LEU  |
| 38  | BP    | 31  | VAL  |
| 38  | BP    | 94  | ALA  |
| 38  | BP    | 110 | LYS  |
| 41  | BS    | 29  | VAL  |
| 42  | BT    | 70  | HIS  |
| 45  | BW    | 75  | ASN  |
| 49  | B0    | 26  | SER  |
| 4   | AE    | 103 | GLY  |
| 7   | AH    | 53  | ASP  |
| 20  | AU    | 3   | ILE  |
| 26  | BD    | 22  | ILE  |
| 26  | BD    | 167 | ASN  |
| 33  | BK    | 2   | ILE  |
| 34  | BL    | 24  | GLY  |
| 35  | BM    | 6   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | BQ    | 32  | ARG  |
| 40  | BR    | 53  | PHE  |
| 42  | BT    | 78  | SER  |
| 44  | BV    | 60  | VAL  |
| 3   | AD    | 27  | ILE  |
| 4   | AE    | 43  | GLY  |
| 42  | BT    | 2   | ILE  |
| 27  | BE    | 96  | VAL  |
| 2   | AC    | 14  | VAL  |
| 4   | AE    | 104 | ILE  |
| 25  | BC    | 108 | GLY  |
| 35  | BM    | 36  | VAL  |
| 38  | BP    | 20  | ARG  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | AB    | 180/180 (100%) | 177 (98%)  | 3 (2%)   | 53          | 69  |
| 2   | AC    | 170/171 (99%)  | 168 (99%)  | 2 (1%)   | 63          | 75  |
| 3   | AD    | 172/173 (99%)  | 171 (99%)  | 1 (1%)   | 78          | 83  |
| 4   | AE    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 5   | AF    | 87/87 (100%)   | 87 (100%)  | 0        | 100         | 100 |
| 6   | AG    | 123/123 (100%) | 123 (100%) | 0        | 100         | 100 |
| 7   | AH    | 104/105 (99%)  | 102 (98%)  | 2 (2%)   | 50          | 67  |
| 8   | AI    | 105/105 (100%) | 105 (100%) | 0        | 100         | 100 |
| 9   | AJ    | 86/86 (100%)   | 83 (96%)   | 3 (4%)   | 32          | 53  |
| 10  | AK    | 90/90 (100%)   | 86 (96%)   | 4 (4%)   | 25          | 47  |
| 11  | AL    | 103/104 (99%)  | 102 (99%)  | 1 (1%)   | 68          | 78  |
| 12  | AM    | 91/92 (99%)    | 91 (100%)  | 0        | 100         | 100 |
| 13  | AN    | 83/84 (99%)    | 83 (100%)  | 0        | 100         | 100 |
| 14  | AO    | 76/77 (99%)    | 75 (99%)   | 1 (1%)   | 61          | 74  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 15  | AP    | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 16  | AQ    | 74/74 (100%)   | 71 (96%)   | 3 (4%)   | 27          | 49  |
| 17  | AR    | 48/48 (100%)   | 47 (98%)   | 1 (2%)   | 47          | 65  |
| 18  | AS    | 70/70 (100%)   | 70 (100%)  | 0        | 100         | 100 |
| 19  | AT    | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 20  | AU    | 44/44 (100%)   | 44 (100%)  | 0        | 100         | 100 |
| 25  | BC    | 216/217 (100%) | 213 (99%)  | 3 (1%)   | 59          | 72  |
| 26  | BD    | 164/164 (100%) | 162 (99%)  | 2 (1%)   | 63          | 75  |
| 27  | BE    | 165/165 (100%) | 163 (99%)  | 2 (1%)   | 63          | 75  |
| 28  | BF    | 149/150 (99%)  | 143 (96%)  | 6 (4%)   | 28          | 49  |
| 29  | BG    | 137/138 (99%)  | 134 (98%)  | 3 (2%)   | 45          | 64  |
| 30  | BH    | 114/114 (100%) | 114 (100%) | 0        | 100         | 100 |
| 31  | BI    | 109/110 (99%)  | 107 (98%)  | 2 (2%)   | 51          | 68  |
| 32  | BJ    | 116/116 (100%) | 114 (98%)  | 2 (2%)   | 53          | 69  |
| 33  | BK    | 103/103 (100%) | 102 (99%)  | 1 (1%)   | 68          | 78  |
| 34  | BL    | 102/103 (99%)  | 102 (100%) | 0        | 100         | 100 |
| 35  | BM    | 109/109 (100%) | 107 (98%)  | 2 (2%)   | 51          | 68  |
| 36  | BN    | 100/100 (100%) | 98 (98%)   | 2 (2%)   | 48          | 66  |
| 37  | BO    | 86/87 (99%)    | 86 (100%)  | 0        | 100         | 100 |
| 38  | BP    | 99/100 (99%)   | 98 (99%)   | 1 (1%)   | 68          | 78  |
| 39  | BQ    | 89/90 (99%)    | 89 (100%)  | 0        | 100         | 100 |
| 40  | BR    | 84/84 (100%)   | 83 (99%)   | 1 (1%)   | 63          | 75  |
| 41  | BS    | 93/93 (100%)   | 92 (99%)   | 1 (1%)   | 65          | 76  |
| 42  | BT    | 80/80 (100%)   | 80 (100%)  | 0        | 100         | 100 |
| 43  | BU    | 83/84 (99%)    | 81 (98%)   | 2 (2%)   | 43          | 64  |
| 44  | BV    | 78/78 (100%)   | 77 (99%)   | 1 (1%)   | 61          | 74  |
| 45  | BW    | 59/59 (100%)   | 59 (100%)  | 0        | 100         | 100 |
| 46  | BX    | 67/68 (98%)    | 66 (98%)   | 1 (2%)   | 57          | 72  |
| 47  | BY    | 55/55 (100%)   | 54 (98%)   | 1 (2%)   | 51          | 68  |
| 48  | BZ    | 48/49 (98%)    | 48 (100%)  | 0        | 100         | 100 |
| 49  | B0    | 47/48 (98%)    | 45 (96%)   | 2 (4%)   | 26          | 47  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 50  | B1    | 45/45 (100%)    | 45 (100%)  | 0        | 100         | 100 |
| 51  | B2    | 38/38 (100%)    | 38 (100%)  | 0        | 100         | 100 |
| 52  | B3    | 51/52 (98%)     | 51 (100%)  | 0        | 100         | 100 |
| 53  | B4    | 34/34 (100%)    | 34 (100%)  | 0        | 100         | 100 |
| 56  | B5    | 173/181 (96%)   | 170 (98%)  | 3 (2%)   | 53          | 69  |
| All | All   | 4842/4870 (99%) | 4783 (99%) | 59 (1%)  | 61          | 75  |

All (59) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AB    | 22  | TRP  |
| 1   | AB    | 88  | GLN  |
| 1   | AB    | 169 | HIS  |
| 2   | AC    | 182 | ASP  |
| 2   | AC    | 187 | GLU  |
| 3   | AD    | 54  | LEU  |
| 7   | AH    | 60  | LEU  |
| 7   | AH    | 86  | LYS  |
| 9   | AJ    | 92  | LEU  |
| 9   | AJ    | 99  | GLN  |
| 9   | AJ    | 102 | LEU  |
| 10  | AK    | 19  | VAL  |
| 10  | AK    | 37  | GLN  |
| 10  | AK    | 80  | ASN  |
| 10  | AK    | 86  | LYS  |
| 11  | AL    | 93  | ARG  |
| 14  | AO    | 20  | ASP  |
| 16  | AQ    | 42  | LYS  |
| 16  | AQ    | 46  | HIS  |
| 16  | AQ    | 69  | THR  |
| 17  | AR    | 70  | THR  |
| 25  | BC    | 62  | ARG  |
| 25  | BC    | 173 | LEU  |
| 25  | BC    | 190 | THR  |
| 26  | BD    | 86  | GLU  |
| 26  | BD    | 151 | THR  |
| 27  | BE    | 17  | THR  |
| 27  | BE    | 77  | ILE  |
| 28  | BF    | 4   | HIS  |
| 28  | BF    | 21  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | BF    | 41  | GLU  |
| 28  | BF    | 49  | LEU  |
| 28  | BF    | 89  | THR  |
| 28  | BF    | 173 | ASP  |
| 29  | BG    | 115 | GLN  |
| 29  | BG    | 154 | GLU  |
| 29  | BG    | 166 | GLU  |
| 31  | BI    | 35  | MET  |
| 31  | BI    | 131 | THR  |
| 32  | BJ    | 50  | THR  |
| 32  | BJ    | 84  | ILE  |
| 33  | BK    | 105 | ARG  |
| 35  | BM    | 108 | VAL  |
| 35  | BM    | 126 | ILE  |
| 36  | BN    | 1   | MET  |
| 36  | BN    | 97  | ILE  |
| 38  | BP    | 64  | SER  |
| 40  | BR    | 94  | THR  |
| 41  | BS    | 74  | ILE  |
| 43  | BU    | 42  | LYS  |
| 43  | BU    | 61  | GLU  |
| 44  | BV    | 12  | GLN  |
| 46  | BX    | 13  | THR  |
| 47  | BY    | 43  | LEU  |
| 49  | B0    | 40  | HIS  |
| 49  | B0    | 54  | ILE  |
| 56  | B5    | 79  | THR  |
| 56  | B5    | 171 | ILE  |
| 56  | B5    | 173 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AB    | 35  | ASN  |
| 1   | AB    | 108 | GLN  |
| 1   | AB    | 169 | HIS  |
| 1   | AB    | 202 | ASN  |
| 2   | AC    | 138 | GLN  |
| 3   | AD    | 70  | GLN  |
| 3   | AD    | 135 | GLN  |
| 5   | AF    | 55  | HIS  |
| 5   | AF    | 81  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | AG    | 51  | GLN  |
| 7   | AH    | 66  | GLN  |
| 8   | AI    | 4   | GLN  |
| 10  | AK    | 21  | HIS  |
| 10  | AK    | 23  | HIS  |
| 10  | AK    | 80  | ASN  |
| 11  | AL    | 4   | ASN  |
| 11  | AL    | 72  | ASN  |
| 13  | AN    | 35  | ASN  |
| 15  | AP    | 26  | ASN  |
| 18  | AS    | 42  | ASN  |
| 19  | AT    | 12  | GLN  |
| 25  | BC    | 24  | HIS  |
| 25  | BC    | 152 | GLN  |
| 25  | BC    | 162 | GLN  |
| 26  | BD    | 58  | ASN  |
| 26  | BD    | 67  | HIS  |
| 26  | BD    | 167 | ASN  |
| 27  | BE    | 62  | GLN  |
| 28  | BF    | 4   | HIS  |
| 29  | BG    | 21  | GLN  |
| 29  | BG    | 44  | HIS  |
| 29  | BG    | 103 | ASN  |
| 29  | BG    | 142 | GLN  |
| 30  | BH    | 2   | GLN  |
| 31  | BI    | 18  | ASN  |
| 31  | BI    | 42  | ASN  |
| 32  | BJ    | 131 | ASN  |
| 32  | BJ    | 138 | GLN  |
| 36  | BN    | 3   | HIS  |
| 36  | BN    | 11  | ASN  |
| 40  | BR    | 12  | HIS  |
| 40  | BR    | 87  | GLN  |
| 41  | BS    | 9   | HIS  |
| 42  | BT    | 59  | ASN  |
| 42  | BT    | 72  | GLN  |
| 42  | BT    | 91  | GLN  |
| 44  | BV    | 44  | HIS  |
| 46  | BX    | 15  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 21  | AA    | 1530/1533 (99%) | 268 (17%)         | 85 (5%)         |
| 22  | A1    | 75/76 (98%)     | 14 (18%)          | 8 (10%)         |
| 23  | A2    | 14/15 (93%)     | 5 (35%)           | 2 (14%)         |
| 24  | A3    | 76/77 (98%)     | 18 (23%)          | 6 (7%)          |
| 54  | BA    | 2902/2903 (99%) | 515 (17%)         | 135 (4%)        |
| 55  | BB    | 116/118 (98%)   | 18 (15%)          | 3 (2%)          |
| All | All   | 4713/4722 (99%) | 838 (17%)         | 239 (5%)        |

All (838) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 6   | G    |
| 21  | AA    | 9   | G    |
| 21  | AA    | 20  | U    |
| 21  | AA    | 21  | G    |
| 21  | AA    | 30  | U    |
| 21  | AA    | 31  | G    |
| 21  | AA    | 32  | A    |
| 21  | AA    | 33  | A    |
| 21  | AA    | 36  | C    |
| 21  | AA    | 39  | G    |
| 21  | AA    | 47  | C    |
| 21  | AA    | 48  | C    |
| 21  | AA    | 49  | U    |
| 21  | AA    | 50  | A    |
| 21  | AA    | 51  | A    |
| 21  | AA    | 61  | G    |
| 21  | AA    | 72  | A    |
| 21  | AA    | 84  | U    |
| 21  | AA    | 85  | U    |
| 21  | AA    | 86  | G    |
| 21  | AA    | 87  | C    |
| 21  | AA    | 94  | G    |
| 21  | AA    | 95  | C    |
| 21  | AA    | 98  | A    |
| 21  | AA    | 99  | C    |
| 21  | AA    | 100 | G    |
| 21  | AA    | 110 | C    |
| 21  | AA    | 112 | G    |
| 21  | AA    | 120 | A    |
| 21  | AA    | 121 | U    |
| 21  | AA    | 125 | U    |
| 21  | AA    | 151 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 153 | C    |
| 21  | AA    | 161 | A    |
| 21  | AA    | 163 | C    |
| 21  | AA    | 164 | G    |
| 21  | AA    | 165 | G    |
| 21  | AA    | 183 | C    |
| 21  | AA    | 184 | G    |
| 21  | AA    | 185 | U    |
| 21  | AA    | 198 | G    |
| 21  | AA    | 201 | G    |
| 21  | AA    | 212 | G    |
| 21  | AA    | 235 | C    |
| 21  | AA    | 240 | G    |
| 21  | AA    | 244 | U    |
| 21  | AA    | 245 | U    |
| 21  | AA    | 247 | G    |
| 21  | AA    | 251 | G    |
| 21  | AA    | 255 | G    |
| 21  | AA    | 256 | U    |
| 21  | AA    | 266 | G    |
| 21  | AA    | 272 | C    |
| 21  | AA    | 289 | G    |
| 21  | AA    | 293 | G    |
| 21  | AA    | 294 | U    |
| 21  | AA    | 298 | A    |
| 21  | AA    | 301 | G    |
| 21  | AA    | 328 | C    |
| 21  | AA    | 330 | C    |
| 21  | AA    | 332 | G    |
| 21  | AA    | 344 | A    |
| 21  | AA    | 345 | C    |
| 21  | AA    | 346 | G    |
| 21  | AA    | 352 | C    |
| 21  | AA    | 353 | A    |
| 21  | AA    | 354 | G    |
| 21  | AA    | 358 | U    |
| 21  | AA    | 365 | U    |
| 21  | AA    | 372 | C    |
| 21  | AA    | 381 | C    |
| 21  | AA    | 384 | G    |
| 21  | AA    | 385 | C    |
| 21  | AA    | 389 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 398 | U    |
| 21  | AA    | 406 | G    |
| 21  | AA    | 412 | A    |
| 21  | AA    | 413 | G    |
| 21  | AA    | 414 | A    |
| 21  | AA    | 415 | A    |
| 21  | AA    | 421 | U    |
| 21  | AA    | 422 | C    |
| 21  | AA    | 424 | G    |
| 21  | AA    | 429 | U    |
| 21  | AA    | 452 | A    |
| 21  | AA    | 457 | G    |
| 21  | AA    | 463 | U    |
| 21  | AA    | 465 | A    |
| 21  | AA    | 466 | A    |
| 21  | AA    | 467 | U    |
| 21  | AA    | 468 | A    |
| 21  | AA    | 474 | G    |
| 21  | AA    | 482 | A    |
| 21  | AA    | 483 | C    |
| 21  | AA    | 484 | G    |
| 21  | AA    | 493 | A    |
| 21  | AA    | 495 | A    |
| 21  | AA    | 497 | G    |
| 21  | AA    | 509 | A    |
| 21  | AA    | 511 | C    |
| 21  | AA    | 524 | G    |
| 21  | AA    | 527 | G    |
| 21  | AA    | 532 | A    |
| 21  | AA    | 547 | A    |
| 21  | AA    | 559 | A    |
| 21  | AA    | 562 | U    |
| 21  | AA    | 566 | G    |
| 21  | AA    | 572 | A    |
| 21  | AA    | 573 | A    |
| 21  | AA    | 576 | C    |
| 21  | AA    | 580 | C    |
| 21  | AA    | 611 | C    |
| 21  | AA    | 612 | C    |
| 21  | AA    | 618 | C    |
| 21  | AA    | 619 | U    |
| 21  | AA    | 620 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 622 | A    |
| 21  | AA    | 623 | C    |
| 21  | AA    | 627 | G    |
| 21  | AA    | 632 | U    |
| 21  | AA    | 641 | U    |
| 21  | AA    | 642 | A    |
| 21  | AA    | 653 | U    |
| 21  | AA    | 661 | G    |
| 21  | AA    | 664 | G    |
| 21  | AA    | 665 | A    |
| 21  | AA    | 687 | A    |
| 21  | AA    | 695 | A    |
| 21  | AA    | 700 | G    |
| 21  | AA    | 724 | G    |
| 21  | AA    | 753 | A    |
| 21  | AA    | 755 | G    |
| 21  | AA    | 777 | A    |
| 21  | AA    | 787 | A    |
| 21  | AA    | 794 | A    |
| 21  | AA    | 812 | G    |
| 21  | AA    | 816 | A    |
| 21  | AA    | 817 | C    |
| 21  | AA    | 819 | A    |
| 21  | AA    | 828 | U    |
| 21  | AA    | 841 | C    |
| 21  | AA    | 843 | U    |
| 21  | AA    | 844 | G    |
| 21  | AA    | 845 | A    |
| 21  | AA    | 846 | G    |
| 21  | AA    | 885 | G    |
| 21  | AA    | 900 | A    |
| 21  | AA    | 926 | G    |
| 21  | AA    | 927 | G    |
| 21  | AA    | 932 | C    |
| 21  | AA    | 933 | G    |
| 21  | AA    | 937 | A    |
| 21  | AA    | 939 | G    |
| 21  | AA    | 945 | G    |
| 21  | AA    | 946 | A    |
| 21  | AA    | 959 | A    |
| 21  | AA    | 960 | U    |
| 21  | AA    | 962 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 965  | U    |
| 21  | AA    | 966  | G    |
| 21  | AA    | 969  | A    |
| 21  | AA    | 971  | G    |
| 21  | AA    | 974  | A    |
| 21  | AA    | 976  | G    |
| 21  | AA    | 977  | A    |
| 21  | AA    | 978  | A    |
| 21  | AA    | 980  | C    |
| 21  | AA    | 983  | A    |
| 21  | AA    | 984  | C    |
| 21  | AA    | 993  | G    |
| 21  | AA    | 994  | A    |
| 21  | AA    | 995  | C    |
| 21  | AA    | 996  | A    |
| 21  | AA    | 997  | U    |
| 21  | AA    | 1004 | A    |
| 21  | AA    | 1020 | G    |
| 21  | AA    | 1031 | C    |
| 21  | AA    | 1032 | G    |
| 21  | AA    | 1033 | G    |
| 21  | AA    | 1045 | C    |
| 21  | AA    | 1050 | G    |
| 21  | AA    | 1051 | C    |
| 21  | AA    | 1056 | U    |
| 21  | AA    | 1060 | U    |
| 21  | AA    | 1061 | G    |
| 21  | AA    | 1068 | G    |
| 21  | AA    | 1081 | A    |
| 21  | AA    | 1094 | G    |
| 21  | AA    | 1095 | U    |
| 21  | AA    | 1101 | A    |
| 21  | AA    | 1102 | A    |
| 21  | AA    | 1136 | C    |
| 21  | AA    | 1137 | C    |
| 21  | AA    | 1139 | G    |
| 21  | AA    | 1140 | C    |
| 21  | AA    | 1141 | C    |
| 21  | AA    | 1142 | G    |
| 21  | AA    | 1143 | G    |
| 21  | AA    | 1151 | A    |
| 21  | AA    | 1157 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 1158 | C    |
| 21  | AA    | 1159 | U    |
| 21  | AA    | 1160 | G    |
| 21  | AA    | 1161 | C    |
| 21  | AA    | 1167 | A    |
| 21  | AA    | 1168 | U    |
| 21  | AA    | 1169 | A    |
| 21  | AA    | 1178 | G    |
| 21  | AA    | 1183 | U    |
| 21  | AA    | 1189 | U    |
| 21  | AA    | 1191 | A    |
| 21  | AA    | 1194 | U    |
| 21  | AA    | 1195 | C    |
| 21  | AA    | 1196 | A    |
| 21  | AA    | 1202 | U    |
| 21  | AA    | 1204 | A    |
| 21  | AA    | 1213 | A    |
| 21  | AA    | 1214 | C    |
| 21  | AA    | 1215 | G    |
| 21  | AA    | 1225 | A    |
| 21  | AA    | 1226 | C    |
| 21  | AA    | 1227 | A    |
| 21  | AA    | 1228 | C    |
| 21  | AA    | 1229 | A    |
| 21  | AA    | 1256 | A    |
| 21  | AA    | 1257 | A    |
| 21  | AA    | 1267 | C    |
| 21  | AA    | 1268 | G    |
| 21  | AA    | 1274 | A    |
| 21  | AA    | 1285 | A    |
| 21  | AA    | 1287 | A    |
| 21  | AA    | 1296 | C    |
| 21  | AA    | 1297 | G    |
| 21  | AA    | 1299 | A    |
| 21  | AA    | 1300 | G    |
| 21  | AA    | 1303 | C    |
| 21  | AA    | 1305 | G    |
| 21  | AA    | 1308 | U    |
| 21  | AA    | 1309 | G    |
| 21  | AA    | 1317 | C    |
| 21  | AA    | 1320 | C    |
| 21  | AA    | 1321 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 1323 | G    |
| 21  | AA    | 1337 | G    |
| 21  | AA    | 1338 | G    |
| 21  | AA    | 1339 | A    |
| 21  | AA    | 1342 | C    |
| 21  | AA    | 1343 | G    |
| 21  | AA    | 1345 | U    |
| 21  | AA    | 1355 | G    |
| 21  | AA    | 1356 | G    |
| 21  | AA    | 1362 | A    |
| 21  | AA    | 1379 | G    |
| 21  | AA    | 1380 | U    |
| 21  | AA    | 1381 | U    |
| 21  | AA    | 1383 | C    |
| 21  | AA    | 1384 | C    |
| 21  | AA    | 1399 | C    |
| 21  | AA    | 1401 | G    |
| 21  | AA    | 1446 | A    |
| 21  | AA    | 1471 | U    |
| 21  | AA    | 1472 | U    |
| 21  | AA    | 1493 | A    |
| 21  | AA    | 1517 | G    |
| 21  | AA    | 1520 | C    |
| 21  | AA    | 1529 | G    |
| 21  | AA    | 1530 | G    |
| 21  | AA    | 1534 | A    |
| 22  | A1    | 10   | G    |
| 22  | A1    | 17   | U    |
| 22  | A1    | 21   | A    |
| 22  | A1    | 32   | C    |
| 22  | A1    | 48   | C    |
| 22  | A1    | 49   | G    |
| 22  | A1    | 56   | C    |
| 22  | A1    | 57   | G    |
| 22  | A1    | 58   | A    |
| 22  | A1    | 60   | C    |
| 22  | A1    | 61   | C    |
| 22  | A1    | 62   | C    |
| 22  | A1    | 73   | A    |
| 22  | A1    | 74   | C    |
| 23  | A2    | 81   | U    |
| 23  | A2    | 82   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | A2    | 83  | U    |
| 23  | A2    | 91  | A    |
| 23  | A2    | 92  | U    |
| 24  | A3    | 2   | G    |
| 24  | A3    | 9   | G    |
| 24  | A3    | 15  | G    |
| 24  | A3    | 16  | C    |
| 24  | A3    | 17  | C    |
| 24  | A3    | 18  | U    |
| 24  | A3    | 19  | G    |
| 24  | A3    | 20  | G    |
| 24  | A3    | 22  | A    |
| 24  | A3    | 48  | U    |
| 24  | A3    | 49  | C    |
| 24  | A3    | 55  | 5MU  |
| 24  | A3    | 56  | PSU  |
| 24  | A3    | 60  | A    |
| 24  | A3    | 73  | A    |
| 24  | A3    | 74  | A    |
| 24  | A3    | 75  | C    |
| 24  | A3    | 76  | C    |
| 54  | BA    | 10  | A    |
| 54  | BA    | 13  | A    |
| 54  | BA    | 14  | A    |
| 54  | BA    | 15  | G    |
| 54  | BA    | 22  | C    |
| 54  | BA    | 43  | G    |
| 54  | BA    | 44  | A    |
| 54  | BA    | 45  | G    |
| 54  | BA    | 46  | G    |
| 54  | BA    | 47  | C    |
| 54  | BA    | 48  | G    |
| 54  | BA    | 52  | A    |
| 54  | BA    | 60  | G    |
| 54  | BA    | 61  | C    |
| 54  | BA    | 62  | U    |
| 54  | BA    | 74  | A    |
| 54  | BA    | 75  | G    |
| 54  | BA    | 77  | G    |
| 54  | BA    | 91  | A    |
| 54  | BA    | 99  | U    |
| 54  | BA    | 100 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | BA    | 101 | A    |
| 54  | BA    | 102 | U    |
| 54  | BA    | 103 | A    |
| 54  | BA    | 119 | A    |
| 54  | BA    | 120 | U    |
| 54  | BA    | 125 | A    |
| 54  | BA    | 126 | A    |
| 54  | BA    | 127 | A    |
| 54  | BA    | 128 | C    |
| 54  | BA    | 142 | A    |
| 54  | BA    | 147 | C    |
| 54  | BA    | 148 | U    |
| 54  | BA    | 155 | A    |
| 54  | BA    | 173 | A    |
| 54  | BA    | 194 | G    |
| 54  | BA    | 196 | A    |
| 54  | BA    | 197 | A    |
| 54  | BA    | 199 | A    |
| 54  | BA    | 200 | U    |
| 54  | BA    | 204 | A    |
| 54  | BA    | 205 | G    |
| 54  | BA    | 216 | A    |
| 54  | BA    | 222 | A    |
| 54  | BA    | 230 | G    |
| 54  | BA    | 233 | A    |
| 54  | BA    | 244 | A    |
| 54  | BA    | 248 | G    |
| 54  | BA    | 249 | C    |
| 54  | BA    | 250 | G    |
| 54  | BA    | 258 | G    |
| 54  | BA    | 265 | A    |
| 54  | BA    | 266 | G    |
| 54  | BA    | 278 | A    |
| 54  | BA    | 279 | A    |
| 54  | BA    | 280 | U    |
| 54  | BA    | 299 | A    |
| 54  | BA    | 301 | G    |
| 54  | BA    | 302 | C    |
| 54  | BA    | 316 | C    |
| 54  | BA    | 322 | A    |
| 54  | BA    | 323 | C    |
| 54  | BA    | 329 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | BA    | 330 | A    |
| 54  | BA    | 331 | C    |
| 54  | BA    | 346 | A    |
| 54  | BA    | 370 | G    |
| 54  | BA    | 371 | A    |
| 54  | BA    | 373 | U    |
| 54  | BA    | 374 | A    |
| 54  | BA    | 386 | G    |
| 54  | BA    | 387 | U    |
| 54  | BA    | 388 | G    |
| 54  | BA    | 389 | G    |
| 54  | BA    | 404 | A    |
| 54  | BA    | 411 | G    |
| 54  | BA    | 428 | A    |
| 54  | BA    | 443 | A    |
| 54  | BA    | 446 | G    |
| 54  | BA    | 447 | A    |
| 54  | BA    | 448 | U    |
| 54  | BA    | 451 | U    |
| 54  | BA    | 457 | A    |
| 54  | BA    | 458 | G    |
| 54  | BA    | 474 | G    |
| 54  | BA    | 475 | C    |
| 54  | BA    | 481 | G    |
| 54  | BA    | 482 | A    |
| 54  | BA    | 491 | G    |
| 54  | BA    | 504 | A    |
| 54  | BA    | 509 | C    |
| 54  | BA    | 512 | G    |
| 54  | BA    | 527 | C    |
| 54  | BA    | 529 | A    |
| 54  | BA    | 530 | G    |
| 54  | BA    | 531 | C    |
| 54  | BA    | 532 | A    |
| 54  | BA    | 533 | G    |
| 54  | BA    | 544 | C    |
| 54  | BA    | 546 | U    |
| 54  | BA    | 548 | G    |
| 54  | BA    | 549 | G    |
| 54  | BA    | 550 | C    |
| 54  | BA    | 573 | U    |
| 54  | BA    | 574 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | BA    | 575 | A    |
| 54  | BA    | 577 | G    |
| 54  | BA    | 579 | G    |
| 54  | BA    | 590 | A    |
| 54  | BA    | 603 | A    |
| 54  | BA    | 613 | A    |
| 54  | BA    | 614 | A    |
| 54  | BA    | 615 | U    |
| 54  | BA    | 637 | A    |
| 54  | BA    | 647 | G    |
| 54  | BA    | 653 | U    |
| 54  | BA    | 654 | A    |
| 54  | BA    | 671 | C    |
| 54  | BA    | 672 | C    |
| 54  | BA    | 686 | U    |
| 54  | BA    | 719 | C    |
| 54  | BA    | 725 | G    |
| 54  | BA    | 726 | G    |
| 54  | BA    | 727 | A    |
| 54  | BA    | 730 | A    |
| 54  | BA    | 736 | C    |
| 54  | BA    | 747 | U    |
| 54  | BA    | 748 | G    |
| 54  | BA    | 751 | A    |
| 54  | BA    | 752 | A    |
| 54  | BA    | 764 | A    |
| 54  | BA    | 775 | G    |
| 54  | BA    | 776 | G    |
| 54  | BA    | 782 | A    |
| 54  | BA    | 784 | G    |
| 54  | BA    | 790 | U    |
| 54  | BA    | 792 | A    |
| 54  | BA    | 805 | G    |
| 54  | BA    | 806 | C    |
| 54  | BA    | 810 | U    |
| 54  | BA    | 812 | C    |
| 54  | BA    | 827 | U    |
| 54  | BA    | 828 | U    |
| 54  | BA    | 847 | U    |
| 54  | BA    | 858 | G    |
| 54  | BA    | 866 | A    |
| 54  | BA    | 889 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 890  | C    |
| 54  | BA    | 907  | G    |
| 54  | BA    | 910  | A    |
| 54  | BA    | 914  | G    |
| 54  | BA    | 915  | C    |
| 54  | BA    | 932  | U    |
| 54  | BA    | 933  | A    |
| 54  | BA    | 946  | C    |
| 54  | BA    | 957  | C    |
| 54  | BA    | 958  | U    |
| 54  | BA    | 959  | A    |
| 54  | BA    | 961  | C    |
| 54  | BA    | 962  | G    |
| 54  | BA    | 965  | C    |
| 54  | BA    | 966  | G    |
| 54  | BA    | 974  | G    |
| 54  | BA    | 983  | A    |
| 54  | BA    | 984  | A    |
| 54  | BA    | 989  | G    |
| 54  | BA    | 990  | A    |
| 54  | BA    | 994  | C    |
| 54  | BA    | 995  | C    |
| 54  | BA    | 996  | A    |
| 54  | BA    | 1012 | U    |
| 54  | BA    | 1013 | C    |
| 54  | BA    | 1024 | G    |
| 54  | BA    | 1025 | G    |
| 54  | BA    | 1026 | G    |
| 54  | BA    | 1033 | U    |
| 54  | BA    | 1046 | A    |
| 54  | BA    | 1047 | G    |
| 54  | BA    | 1063 | G    |
| 54  | BA    | 1068 | G    |
| 54  | BA    | 1070 | A    |
| 54  | BA    | 1071 | G    |
| 54  | BA    | 1073 | A    |
| 54  | BA    | 1088 | A    |
| 54  | BA    | 1089 | A    |
| 54  | BA    | 1090 | A    |
| 54  | BA    | 1095 | A    |
| 54  | BA    | 1096 | A    |
| 54  | BA    | 1097 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 1102 | C    |
| 54  | BA    | 1112 | G    |
| 54  | BA    | 1127 | A    |
| 54  | BA    | 1129 | A    |
| 54  | BA    | 1132 | U    |
| 54  | BA    | 1133 | A    |
| 54  | BA    | 1134 | A    |
| 54  | BA    | 1135 | C    |
| 54  | BA    | 1142 | A    |
| 54  | BA    | 1144 | A    |
| 54  | BA    | 1155 | A    |
| 54  | BA    | 1176 | U    |
| 54  | BA    | 1177 | G    |
| 54  | BA    | 1185 | G    |
| 54  | BA    | 1186 | G    |
| 54  | BA    | 1189 | A    |
| 54  | BA    | 1204 | A    |
| 54  | BA    | 1211 | C    |
| 54  | BA    | 1227 | G    |
| 54  | BA    | 1236 | G    |
| 54  | BA    | 1237 | A    |
| 54  | BA    | 1241 | A    |
| 54  | BA    | 1242 | U    |
| 54  | BA    | 1252 | G    |
| 54  | BA    | 1253 | A    |
| 54  | BA    | 1254 | A    |
| 54  | BA    | 1255 | U    |
| 54  | BA    | 1256 | G    |
| 54  | BA    | 1262 | A    |
| 54  | BA    | 1263 | U    |
| 54  | BA    | 1266 | G    |
| 54  | BA    | 1272 | A    |
| 54  | BA    | 1273 | U    |
| 54  | BA    | 1274 | A    |
| 54  | BA    | 1275 | A    |
| 54  | BA    | 1276 | A    |
| 54  | BA    | 1287 | A    |
| 54  | BA    | 1300 | G    |
| 54  | BA    | 1301 | A    |
| 54  | BA    | 1302 | A    |
| 54  | BA    | 1303 | G    |
| 54  | BA    | 1311 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 1312 | U    |
| 54  | BA    | 1313 | U    |
| 54  | BA    | 1328 | A    |
| 54  | BA    | 1332 | G    |
| 54  | BA    | 1341 | G    |
| 54  | BA    | 1342 | A    |
| 54  | BA    | 1350 | C    |
| 54  | BA    | 1365 | A    |
| 54  | BA    | 1366 | A    |
| 54  | BA    | 1379 | U    |
| 54  | BA    | 1380 | G    |
| 54  | BA    | 1384 | A    |
| 54  | BA    | 1385 | A    |
| 54  | BA    | 1386 | C    |
| 54  | BA    | 1388 | G    |
| 54  | BA    | 1390 | U    |
| 54  | BA    | 1396 | U    |
| 54  | BA    | 1416 | G    |
| 54  | BA    | 1417 | C    |
| 54  | BA    | 1420 | A    |
| 54  | BA    | 1427 | A    |
| 54  | BA    | 1428 | C    |
| 54  | BA    | 1440 | U    |
| 54  | BA    | 1452 | G    |
| 54  | BA    | 1453 | A    |
| 54  | BA    | 1454 | C    |
| 54  | BA    | 1455 | G    |
| 54  | BA    | 1459 | G    |
| 54  | BA    | 1460 | U    |
| 54  | BA    | 1461 | C    |
| 54  | BA    | 1482 | G    |
| 54  | BA    | 1490 | A    |
| 54  | BA    | 1491 | G    |
| 54  | BA    | 1493 | C    |
| 54  | BA    | 1508 | A    |
| 54  | BA    | 1509 | A    |
| 54  | BA    | 1523 | U    |
| 54  | BA    | 1538 | G    |
| 54  | BA    | 1539 | U    |
| 54  | BA    | 1540 | G    |
| 54  | BA    | 1568 | G    |
| 54  | BA    | 1569 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 1574 | C    |
| 54  | BA    | 1578 | U    |
| 54  | BA    | 1585 | C    |
| 54  | BA    | 1586 | A    |
| 54  | BA    | 1598 | A    |
| 54  | BA    | 1599 | U    |
| 54  | BA    | 1604 | C    |
| 54  | BA    | 1608 | A    |
| 54  | BA    | 1617 | C    |
| 54  | BA    | 1618 | A    |
| 54  | BA    | 1621 | U    |
| 54  | BA    | 1622 | G    |
| 54  | BA    | 1626 | A    |
| 54  | BA    | 1635 | A    |
| 54  | BA    | 1639 | C    |
| 54  | BA    | 1646 | C    |
| 54  | BA    | 1647 | U    |
| 54  | BA    | 1648 | U    |
| 54  | BA    | 1650 | A    |
| 54  | BA    | 1653 | G    |
| 54  | BA    | 1654 | A    |
| 54  | BA    | 1663 | G    |
| 54  | BA    | 1666 | G    |
| 54  | BA    | 1668 | A    |
| 54  | BA    | 1669 | A    |
| 54  | BA    | 1674 | G    |
| 54  | BA    | 1707 | G    |
| 54  | BA    | 1729 | U    |
| 54  | BA    | 1737 | G    |
| 54  | BA    | 1738 | G    |
| 54  | BA    | 1758 | U    |
| 54  | BA    | 1764 | C    |
| 54  | BA    | 1773 | A    |
| 54  | BA    | 1783 | A    |
| 54  | BA    | 1784 | A    |
| 54  | BA    | 1785 | A    |
| 54  | BA    | 1800 | C    |
| 54  | BA    | 1804 | C    |
| 54  | BA    | 1808 | A    |
| 54  | BA    | 1811 | G    |
| 54  | BA    | 1819 | A    |
| 54  | BA    | 1820 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 1830 | C    |
| 54  | BA    | 1835 | G    |
| 54  | BA    | 1847 | A    |
| 54  | BA    | 1869 | G    |
| 54  | BA    | 1870 | C    |
| 54  | BA    | 1871 | A    |
| 54  | BA    | 1873 | G    |
| 54  | BA    | 1874 | C    |
| 54  | BA    | 1900 | A    |
| 54  | BA    | 1914 | C    |
| 54  | BA    | 1915 | U    |
| 54  | BA    | 1930 | G    |
| 54  | BA    | 1931 | U    |
| 54  | BA    | 1937 | A    |
| 54  | BA    | 1938 | A    |
| 54  | BA    | 1939 | U    |
| 54  | BA    | 1941 | C    |
| 54  | BA    | 1942 | C    |
| 54  | BA    | 1943 | U    |
| 54  | BA    | 1944 | U    |
| 54  | BA    | 1945 | G    |
| 54  | BA    | 1946 | U    |
| 54  | BA    | 1952 | A    |
| 54  | BA    | 1953 | A    |
| 54  | BA    | 1955 | U    |
| 54  | BA    | 1967 | C    |
| 54  | BA    | 1970 | A    |
| 54  | BA    | 1971 | U    |
| 54  | BA    | 1972 | G    |
| 54  | BA    | 1980 | G    |
| 54  | BA    | 1981 | A    |
| 54  | BA    | 1982 | U    |
| 54  | BA    | 1993 | U    |
| 54  | BA    | 1996 | C    |
| 54  | BA    | 1997 | C    |
| 54  | BA    | 2006 | C    |
| 54  | BA    | 2022 | U    |
| 54  | BA    | 2023 | C    |
| 54  | BA    | 2032 | G    |
| 54  | BA    | 2035 | G    |
| 54  | BA    | 2036 | C    |
| 54  | BA    | 2044 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 2052 | A    |
| 54  | BA    | 2055 | C    |
| 54  | BA    | 2060 | A    |
| 54  | BA    | 2061 | G    |
| 54  | BA    | 2063 | C    |
| 54  | BA    | 2068 | U    |
| 54  | BA    | 2076 | U    |
| 54  | BA    | 2077 | A    |
| 54  | BA    | 2092 | U    |
| 54  | BA    | 2111 | U    |
| 54  | BA    | 2112 | G    |
| 54  | BA    | 2117 | A    |
| 54  | BA    | 2118 | U    |
| 54  | BA    | 2119 | A    |
| 54  | BA    | 2126 | A    |
| 54  | BA    | 2127 | G    |
| 54  | BA    | 2157 | G    |
| 54  | BA    | 2159 | G    |
| 54  | BA    | 2160 | C    |
| 54  | BA    | 2165 | C    |
| 54  | BA    | 2169 | A    |
| 54  | BA    | 2172 | U    |
| 54  | BA    | 2203 | U    |
| 54  | BA    | 2211 | A    |
| 54  | BA    | 2212 | A    |
| 54  | BA    | 2213 | U    |
| 54  | BA    | 2232 | C    |
| 54  | BA    | 2238 | G    |
| 54  | BA    | 2244 | U    |
| 54  | BA    | 2245 | U    |
| 54  | BA    | 2246 | G    |
| 54  | BA    | 2267 | A    |
| 54  | BA    | 2269 | G    |
| 54  | BA    | 2275 | C    |
| 54  | BA    | 2283 | C    |
| 54  | BA    | 2297 | A    |
| 54  | BA    | 2304 | G    |
| 54  | BA    | 2305 | U    |
| 54  | BA    | 2307 | G    |
| 54  | BA    | 2308 | G    |
| 54  | BA    | 2309 | A    |
| 54  | BA    | 2311 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 2312 | U    |
| 54  | BA    | 2313 | C    |
| 54  | BA    | 2320 | U    |
| 54  | BA    | 2321 | U    |
| 54  | BA    | 2325 | G    |
| 54  | BA    | 2326 | C    |
| 54  | BA    | 2333 | A    |
| 54  | BA    | 2334 | U    |
| 54  | BA    | 2335 | A    |
| 54  | BA    | 2347 | C    |
| 54  | BA    | 2353 | G    |
| 54  | BA    | 2383 | G    |
| 54  | BA    | 2385 | C    |
| 54  | BA    | 2388 | A    |
| 54  | BA    | 2389 | G    |
| 54  | BA    | 2390 | U    |
| 54  | BA    | 2391 | G    |
| 54  | BA    | 2392 | A    |
| 54  | BA    | 2394 | C    |
| 54  | BA    | 2407 | A    |
| 54  | BA    | 2424 | C    |
| 54  | BA    | 2425 | A    |
| 54  | BA    | 2426 | A    |
| 54  | BA    | 2428 | G    |
| 54  | BA    | 2429 | G    |
| 54  | BA    | 2431 | U    |
| 54  | BA    | 2432 | A    |
| 54  | BA    | 2433 | A    |
| 54  | BA    | 2434 | A    |
| 54  | BA    | 2439 | A    |
| 54  | BA    | 2440 | C    |
| 54  | BA    | 2441 | U    |
| 54  | BA    | 2447 | G    |
| 54  | BA    | 2448 | A    |
| 54  | BA    | 2449 | U    |
| 54  | BA    | 2473 | U    |
| 54  | BA    | 2474 | U    |
| 54  | BA    | 2478 | A    |
| 54  | BA    | 2483 | C    |
| 54  | BA    | 2484 | G    |
| 54  | BA    | 2485 | G    |
| 54  | BA    | 2491 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 2495 | G    |
| 54  | BA    | 2496 | C    |
| 54  | BA    | 2498 | C    |
| 54  | BA    | 2499 | C    |
| 54  | BA    | 2500 | U    |
| 54  | BA    | 2502 | G    |
| 54  | BA    | 2504 | U    |
| 54  | BA    | 2505 | G    |
| 54  | BA    | 2529 | G    |
| 54  | BA    | 2531 | A    |
| 54  | BA    | 2532 | G    |
| 54  | BA    | 2534 | A    |
| 54  | BA    | 2540 | C    |
| 54  | BA    | 2547 | A    |
| 54  | BA    | 2554 | U    |
| 54  | BA    | 2556 | C    |
| 54  | BA    | 2565 | A    |
| 54  | BA    | 2566 | A    |
| 54  | BA    | 2567 | G    |
| 54  | BA    | 2573 | C    |
| 54  | BA    | 2585 | U    |
| 54  | BA    | 2586 | U    |
| 54  | BA    | 2589 | A    |
| 54  | BA    | 2599 | G    |
| 54  | BA    | 2602 | A    |
| 54  | BA    | 2603 | G    |
| 54  | BA    | 2614 | A    |
| 54  | BA    | 2617 | U    |
| 54  | BA    | 2629 | U    |
| 54  | BA    | 2630 | G    |
| 54  | BA    | 2642 | G    |
| 54  | BA    | 2655 | G    |
| 54  | BA    | 2660 | A    |
| 54  | BA    | 2661 | G    |
| 54  | BA    | 2663 | G    |
| 54  | BA    | 2665 | A    |
| 54  | BA    | 2666 | C    |
| 54  | BA    | 2669 | G    |
| 54  | BA    | 2676 | C    |
| 54  | BA    | 2684 | U    |
| 54  | BA    | 2689 | U    |
| 54  | BA    | 2690 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 2691 | C    |
| 54  | BA    | 2707 | U    |
| 54  | BA    | 2712 | C    |
| 54  | BA    | 2713 | U    |
| 54  | BA    | 2718 | G    |
| 54  | BA    | 2732 | G    |
| 54  | BA    | 2750 | A    |
| 54  | BA    | 2751 | G    |
| 54  | BA    | 2752 | C    |
| 54  | BA    | 2765 | A    |
| 54  | BA    | 2778 | A    |
| 54  | BA    | 2779 | U    |
| 54  | BA    | 2780 | G    |
| 54  | BA    | 2786 | U    |
| 54  | BA    | 2791 | G    |
| 54  | BA    | 2797 | U    |
| 54  | BA    | 2799 | A    |
| 54  | BA    | 2800 | A    |
| 54  | BA    | 2801 | G    |
| 54  | BA    | 2816 | G    |
| 54  | BA    | 2820 | A    |
| 54  | BA    | 2821 | A    |
| 54  | BA    | 2824 | C    |
| 54  | BA    | 2850 | A    |
| 54  | BA    | 2858 | C    |
| 54  | BA    | 2867 | G    |
| 54  | BA    | 2884 | U    |
| 54  | BA    | 2885 | G    |
| 54  | BA    | 2886 | A    |
| 54  | BA    | 2887 | A    |
| 54  | BA    | 2893 | A    |
| 54  | BA    | 2895 | G    |
| 55  | BB    | 9    | G    |
| 55  | BB    | 11   | C    |
| 55  | BB    | 13   | G    |
| 55  | BB    | 14   | U    |
| 55  | BB    | 15   | A    |
| 55  | BB    | 16   | G    |
| 55  | BB    | 24   | G    |
| 55  | BB    | 25   | U    |
| 55  | BB    | 35   | C    |
| 55  | BB    | 36   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | BB    | 37  | C    |
| 55  | BB    | 44  | G    |
| 55  | BB    | 45  | A    |
| 55  | BB    | 57  | A    |
| 55  | BB    | 67  | G    |
| 55  | BB    | 83  | G    |
| 55  | BB    | 89  | U    |
| 55  | BB    | 109 | A    |

All (239) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 5   | U    |
| 21  | AA    | 30  | U    |
| 21  | AA    | 32  | A    |
| 21  | AA    | 49  | U    |
| 21  | AA    | 51  | A    |
| 21  | AA    | 60  | A    |
| 21  | AA    | 85  | U    |
| 21  | AA    | 94  | G    |
| 21  | AA    | 98  | A    |
| 21  | AA    | 109 | A    |
| 21  | AA    | 120 | A    |
| 21  | AA    | 184 | G    |
| 21  | AA    | 234 | C    |
| 21  | AA    | 244 | U    |
| 21  | AA    | 255 | G    |
| 21  | AA    | 293 | G    |
| 21  | AA    | 344 | A    |
| 21  | AA    | 345 | C    |
| 21  | AA    | 351 | G    |
| 21  | AA    | 353 | A    |
| 21  | AA    | 357 | G    |
| 21  | AA    | 384 | G    |
| 21  | AA    | 412 | A    |
| 21  | AA    | 414 | A    |
| 21  | AA    | 465 | A    |
| 21  | AA    | 482 | A    |
| 21  | AA    | 493 | A    |
| 21  | AA    | 559 | A    |
| 21  | AA    | 575 | G    |
| 21  | AA    | 579 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 602  | A    |
| 21  | AA    | 611  | C    |
| 21  | AA    | 622  | A    |
| 21  | AA    | 626  | G    |
| 21  | AA    | 641  | U    |
| 21  | AA    | 664  | G    |
| 21  | AA    | 733  | G    |
| 21  | AA    | 753  | A    |
| 21  | AA    | 804  | U    |
| 21  | AA    | 811  | C    |
| 21  | AA    | 841  | C    |
| 21  | AA    | 872  | A    |
| 21  | AA    | 884  | U    |
| 21  | AA    | 926  | G    |
| 21  | AA    | 932  | C    |
| 21  | AA    | 945  | G    |
| 21  | AA    | 958  | A    |
| 21  | AA    | 975  | A    |
| 21  | AA    | 982  | U    |
| 21  | AA    | 983  | A    |
| 21  | AA    | 992  | U    |
| 21  | AA    | 994  | A    |
| 21  | AA    | 996  | A    |
| 21  | AA    | 1031 | C    |
| 21  | AA    | 1050 | G    |
| 21  | AA    | 1060 | U    |
| 21  | AA    | 1101 | A    |
| 21  | AA    | 1129 | C    |
| 21  | AA    | 1140 | C    |
| 21  | AA    | 1142 | G    |
| 21  | AA    | 1157 | A    |
| 21  | AA    | 1167 | A    |
| 21  | AA    | 1190 | G    |
| 21  | AA    | 1194 | U    |
| 21  | AA    | 1196 | A    |
| 21  | AA    | 1201 | A    |
| 21  | AA    | 1214 | C    |
| 21  | AA    | 1225 | A    |
| 21  | AA    | 1226 | C    |
| 21  | AA    | 1227 | A    |
| 21  | AA    | 1267 | C    |
| 21  | AA    | 1281 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 1296 | C    |
| 21  | AA    | 1298 | U    |
| 21  | AA    | 1299 | A    |
| 21  | AA    | 1308 | U    |
| 21  | AA    | 1319 | A    |
| 21  | AA    | 1322 | C    |
| 21  | AA    | 1338 | G    |
| 21  | AA    | 1342 | C    |
| 21  | AA    | 1355 | G    |
| 21  | AA    | 1380 | U    |
| 21  | AA    | 1383 | C    |
| 21  | AA    | 1399 | C    |
| 21  | AA    | 1471 | U    |
| 22  | A1    | 10   | G    |
| 22  | A1    | 43   | G    |
| 22  | A1    | 48   | C    |
| 22  | A1    | 55   | PSU  |
| 22  | A1    | 57   | G    |
| 22  | A1    | 58   | A    |
| 22  | A1    | 60   | C    |
| 22  | A1    | 61   | C    |
| 23  | A2    | 80   | C    |
| 23  | A2    | 91   | A    |
| 24  | A3    | 15   | G    |
| 24  | A3    | 16   | C    |
| 24  | A3    | 19   | G    |
| 24  | A3    | 48   | U    |
| 24  | A3    | 72   | C    |
| 24  | A3    | 74   | A    |
| 54  | BA    | 9    | G    |
| 54  | BA    | 13   | A    |
| 54  | BA    | 14   | A    |
| 54  | BA    | 43   | G    |
| 54  | BA    | 45   | G    |
| 54  | BA    | 47   | C    |
| 54  | BA    | 60   | G    |
| 54  | BA    | 99   | U    |
| 54  | BA    | 101  | A    |
| 54  | BA    | 118  | A    |
| 54  | BA    | 119  | A    |
| 54  | BA    | 125  | A    |
| 54  | BA    | 127  | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 147  | C    |
| 54  | BA    | 196  | A    |
| 54  | BA    | 199  | A    |
| 54  | BA    | 233  | A    |
| 54  | BA    | 249  | C    |
| 54  | BA    | 278  | A    |
| 54  | BA    | 279  | A    |
| 54  | BA    | 323  | C    |
| 54  | BA    | 330  | A    |
| 54  | BA    | 369  | U    |
| 54  | BA    | 388  | G    |
| 54  | BA    | 443  | A    |
| 54  | BA    | 446  | G    |
| 54  | BA    | 474  | G    |
| 54  | BA    | 481  | G    |
| 54  | BA    | 504  | A    |
| 54  | BA    | 529  | A    |
| 54  | BA    | 530  | G    |
| 54  | BA    | 532  | A    |
| 54  | BA    | 574  | A    |
| 54  | BA    | 614  | A    |
| 54  | BA    | 670  | A    |
| 54  | BA    | 726  | G    |
| 54  | BA    | 762  | U    |
| 54  | BA    | 790  | U    |
| 54  | BA    | 810  | U    |
| 54  | BA    | 827  | U    |
| 54  | BA    | 957  | C    |
| 54  | BA    | 961  | C    |
| 54  | BA    | 965  | C    |
| 54  | BA    | 980  | A    |
| 54  | BA    | 984  | A    |
| 54  | BA    | 989  | G    |
| 54  | BA    | 994  | C    |
| 54  | BA    | 1067 | A    |
| 54  | BA    | 1069 | A    |
| 54  | BA    | 1089 | A    |
| 54  | BA    | 1096 | A    |
| 54  | BA    | 1126 | A    |
| 54  | BA    | 1132 | U    |
| 54  | BA    | 1141 | U    |
| 54  | BA    | 1175 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 1185 | G    |
| 54  | BA    | 1236 | G    |
| 54  | BA    | 1254 | A    |
| 54  | BA    | 1255 | U    |
| 54  | BA    | 1262 | A    |
| 54  | BA    | 1273 | U    |
| 54  | BA    | 1288 | G    |
| 54  | BA    | 1300 | G    |
| 54  | BA    | 1301 | A    |
| 54  | BA    | 1312 | U    |
| 54  | BA    | 1379 | U    |
| 54  | BA    | 1384 | A    |
| 54  | BA    | 1427 | A    |
| 54  | BA    | 1451 | C    |
| 54  | BA    | 1453 | A    |
| 54  | BA    | 1490 | A    |
| 54  | BA    | 1508 | A    |
| 54  | BA    | 1539 | U    |
| 54  | BA    | 1552 | A    |
| 54  | BA    | 1598 | A    |
| 54  | BA    | 1621 | U    |
| 54  | BA    | 1634 | A    |
| 54  | BA    | 1668 | A    |
| 54  | BA    | 1699 | G    |
| 54  | BA    | 1706 | C    |
| 54  | BA    | 1737 | G    |
| 54  | BA    | 1774 | C    |
| 54  | BA    | 1779 | U    |
| 54  | BA    | 1783 | A    |
| 54  | BA    | 1784 | A    |
| 54  | BA    | 1816 | C    |
| 54  | BA    | 1819 | A    |
| 54  | BA    | 1828 | G    |
| 54  | BA    | 1869 | G    |
| 54  | BA    | 1930 | G    |
| 54  | BA    | 1938 | A    |
| 54  | BA    | 1941 | C    |
| 54  | BA    | 1943 | U    |
| 54  | BA    | 1945 | G    |
| 54  | BA    | 1952 | A    |
| 54  | BA    | 1970 | A    |
| 54  | BA    | 1971 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | BA    | 1980 | G    |
| 54  | BA    | 2005 | A    |
| 54  | BA    | 2035 | G    |
| 54  | BA    | 2076 | U    |
| 54  | BA    | 2110 | G    |
| 54  | BA    | 2117 | A    |
| 54  | BA    | 2141 | G    |
| 54  | BA    | 2164 | C    |
| 54  | BA    | 2211 | A    |
| 54  | BA    | 2227 | A    |
| 54  | BA    | 2244 | U    |
| 54  | BA    | 2245 | U    |
| 54  | BA    | 2275 | C    |
| 54  | BA    | 2282 | G    |
| 54  | BA    | 2286 | G    |
| 54  | BA    | 2304 | G    |
| 54  | BA    | 2311 | A    |
| 54  | BA    | 2352 | A    |
| 54  | BA    | 2389 | G    |
| 54  | BA    | 2391 | G    |
| 54  | BA    | 2402 | U    |
| 54  | BA    | 2425 | A    |
| 54  | BA    | 2439 | A    |
| 54  | BA    | 2473 | U    |
| 54  | BA    | 2483 | C    |
| 54  | BA    | 2495 | G    |
| 54  | BA    | 2565 | A    |
| 54  | BA    | 2585 | U    |
| 54  | BA    | 2602 | A    |
| 54  | BA    | 2641 | G    |
| 54  | BA    | 2645 | G    |
| 54  | BA    | 2665 | A    |
| 54  | BA    | 2690 | U    |
| 54  | BA    | 2711 | A    |
| 54  | BA    | 2712 | C    |
| 54  | BA    | 2780 | G    |
| 54  | BA    | 2799 | A    |
| 54  | BA    | 2894 | G    |
| 55  | BB    | 24   | G    |
| 55  | BB    | 56   | G    |
| 55  | BB    | 82   | U    |

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

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

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

| Mol | Type | Chain | Res | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |       | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 24  | 5MU  | A3    | 55  | 24    | 19,22,23     | 0.68 | 0           | 27,32,35    | 1.45 | 5 (18%)     |
| 24  | H2U  | A3    | 21  | 24    | 18,21,22     | 1.34 | 2 (11%)     | 19,30,33    | 1.31 | 3 (15%)     |
| 22  | CM0  | A1    | 34  | 23,22 | 21,26,27     | 1.30 | 2 (9%)      | 26,37,40    | 1.45 | 3 (11%)     |
| 24  | 4SU  | A3    | 8   | 24    | 18,21,22     | 1.46 | 2 (11%)     | 25,30,33    | 0.82 | 1 (4%)      |
| 22  | 7MG  | A1    | 46  | 22    | 23,26,27     | 4.23 | 3 (13%)     | 27,39,42    | 1.54 | 2 (7%)      |
| 22  | 6MZ  | A1    | 37  | 22    | 22,25,26     | 0.66 | 0           | 29,36,39    | 1.13 | 2 (6%)      |
| 22  | 4SU  | A1    | 7   | 22    | 18,21,22     | 1.36 | 2 (11%)     | 25,30,33    | 0.94 | 2 (8%)      |
| 24  | OMC  | A3    | 33  | 24    | 19,22,23     | 0.75 | 0           | 25,31,34    | 1.29 | 2 (8%)      |
| 22  | 5MU  | A1    | 54  | 22    | 19,22,23     | 0.71 | 0           | 27,32,35    | 1.18 | 3 (11%)     |
| 24  | PSU  | A3    | 56  | 24    | 18,21,22     | 0.77 | 0           | 21,30,33    | 1.09 | 2 (9%)      |
| 22  | PSU  | A1    | 55  | 22    | 18,21,22     | 1.34 | 4 (22%)     | 21,30,33    | 1.97 | 7 (33%)     |

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

| Mol | Type | Chain | Res | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|-------|---------|------------|---------|
| 24  | 5MU  | A3    | 55  | 24    | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | H2U  | A3    | 21  | 24    | -       | 0/7/38/39  | 0/2/2/2 |
| 22  | CM0  | A1    | 34  | 23,22 | -       | 2/12/30/31 | 0/2/2/2 |
| 24  | 4SU  | A3    | 8   | 24    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 7MG  | A1    | 46  | 22    | -       | 0/7/37/38  | 0/3/3/3 |
| 22  | 6MZ  | A1    | 37  | 22    | -       | 0/9/27/28  | 0/3/3/3 |
| 22  | 4SU  | A1    | 7   | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | OMC  | A3    | 33  | 24    | -       | 0/9/27/28  | 0/2/2/2 |
| 22  | 5MU  | A1    | 54  | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | PSU  | A3    | 56  | 24    | -       | 2/7/25/26  | 0/2/2/2 |
| 22  | PSU  | A1    | 55  | 22    | -       | 1/7/25/26  | 0/2/2/2 |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 22  | A1    | 46  | 7MG  | C8-N9   | -19.87 | 1.33        | 1.45     |
| 24  | A3    | 8   | 4SU  | C5-C4   | -5.14  | 1.36        | 1.42     |
| 22  | A1    | 7   | 4SU  | C5-C4   | -4.82  | 1.36        | 1.42     |
| 22  | A1    | 34  | CM0  | O5-C5   | -4.78  | 1.25        | 1.36     |
| 24  | A3    | 21  | H2U  | C2-N3   | -3.45  | 1.31        | 1.38     |
| 24  | A3    | 21  | H2U  | C4-N3   | -3.34  | 1.32        | 1.37     |
| 22  | A1    | 55  | PSU  | C2'-C1' | -3.23  | 1.49        | 1.53     |
| 22  | A1    | 55  | PSU  | C1'-C5  | 2.63   | 1.56        | 1.50     |
| 22  | A1    | 46  | 7MG  | C8-N7   | -2.33  | 1.31        | 1.42     |
| 22  | A1    | 34  | CM0  | O8-C8   | -2.22  | 1.23        | 1.30     |
| 22  | A1    | 7   | 4SU  | C4-S4   | -2.19  | 1.64        | 1.68     |
| 22  | A1    | 46  | 7MG  | C5-N7   | 2.18   | 1.38        | 1.35     |
| 22  | A1    | 55  | PSU  | O4'-C1' | -2.17  | 1.40        | 1.43     |
| 24  | A3    | 8   | 4SU  | C4-S4   | -2.10  | 1.65        | 1.68     |
| 22  | A1    | 55  | PSU  | O4'-C4' | -2.03  | 1.40        | 1.45     |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A1    | 46  | 7MG  | N9-C8-N7    | 5.86  | 111.67      | 103.37   |
| 22  | A1    | 34  | CM0  | C7-O5-C5    | 5.21  | 124.12      | 117.48   |
| 22  | A1    | 55  | PSU  | C6-C5-C4    | -4.26 | 115.30      | 118.17   |
| 22  | A1    | 37  | 6MZ  | C9-N6-C6    | 4.11  | 126.66      | 122.85   |
| 24  | A3    | 33  | OMC  | O2-C2-N3    | -3.94 | 116.11      | 122.33   |
| 24  | A3    | 21  | H2U  | N3-C2-N1    | 3.64  | 120.30      | 116.65   |
| 22  | A1    | 55  | PSU  | C5-C6-N1    | -3.51 | 117.27      | 122.14   |
| 22  | A1    | 55  | PSU  | C6-N1-C2    | -3.51 | 119.44      | 122.69   |
| 22  | A1    | 54  | 5MU  | C6-C5-C4    | 3.35  | 120.78      | 118.02   |
| 22  | A1    | 55  | PSU  | O4'-C1'-C2' | 3.03  | 109.35      | 105.15   |
| 24  | A3    | 55  | 5MU  | C6-C5-C4    | 3.01  | 120.50      | 118.02   |
| 24  | A3    | 55  | 5MU  | C5M-C5-C6   | -2.98 | 118.82      | 122.85   |
| 22  | A1    | 55  | PSU  | O2'-C2'-C1' | -2.87 | 104.39      | 111.21   |
| 22  | A1    | 54  | 5MU  | C5M-C5-C6   | -2.74 | 119.14      | 122.85   |
| 24  | A3    | 33  | OMC  | C2'-C1'-N1  | -2.59 | 109.33      | 114.24   |
| 24  | A3    | 21  | H2U  | O2-C2-N3    | -2.48 | 116.91      | 121.49   |
| 22  | A1    | 55  | PSU  | C4-N3-C2    | -2.44 | 123.01      | 126.37   |
| 24  | A3    | 56  | PSU  | C6-C5-C4    | 2.44  | 119.82      | 118.17   |
| 24  | A3    | 55  | 5MU  | O4'-C4'-C3' | 2.44  | 109.99      | 105.15   |
| 24  | A3    | 21  | H2U  | C5-C4-N3    | 2.41  | 119.25      | 116.69   |
| 24  | A3    | 55  | 5MU  | C5-C6-N1    | -2.33 | 120.78      | 123.31   |
| 22  | A1    | 7   | 4SU  | C6-C5-C4    | 2.31  | 121.95      | 119.95   |
| 24  | A3    | 55  | 5MU  | C3'-C2'-C1' | 2.28  | 105.78      | 101.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A1    | 37  | 6MZ  | C4-C5-C6    | -2.25 | 114.91      | 116.78   |
| 22  | A1    | 7   | 4SU  | O4'-C4'-C3' | 2.22  | 109.56      | 105.15   |
| 24  | A3    | 8   | 4SU  | C6-C5-C4    | 2.15  | 121.82      | 119.95   |
| 22  | A1    | 46  | 7MG  | C6-C5-C4    | -2.15 | 118.62      | 122.40   |
| 22  | A1    | 34  | CM0  | O8-C8-O9    | -2.12 | 117.87      | 123.33   |
| 24  | A3    | 56  | PSU  | O4'-C1'-C2' | 2.10  | 108.06      | 105.15   |
| 22  | A1    | 34  | CM0  | O4'-C4'-C3' | 2.09  | 109.30      | 105.15   |
| 22  | A1    | 55  | PSU  | C5-C4-N3    | -2.08 | 111.97      | 116.55   |
| 22  | A1    | 54  | 5MU  | C5-C6-N1    | -2.01 | 121.13      | 123.31   |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 22  | A1    | 55  | PSU  | C2'-C1'-C5-C4 |
| 24  | A3    | 56  | PSU  | O4'-C1'-C5-C4 |
| 24  | A3    | 56  | PSU  | O4'-C1'-C5-C6 |
| 22  | A1    | 34  | CM0  | O5-C7-C8-O8   |
| 22  | A1    | 34  | CM0  | O5-C7-C8-O9   |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | A1    | 55  | PSU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 58  | FME  | A1    | 102 | 57    | 8,9,10       | 0.76 | 0        | 8,9,11      | 2.01 | 3 (37%)  |
| 57  | VAL  | A1    | 101 | 58,22 | 4,6,7        | 0.62 | 0        | 6,7,9       | 1.81 | 1 (16%)  |

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 |
|-----|------|-------|-----|-------|---------|----------|-------|
| 58  | FME  | A1    | 102 | 57    | -       | 1/7/9/11 | -     |
| 57  | VAL  | A1    | 101 | 58,22 | -       | 0/5/6/8  | -     |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 57  | A1    | 101 | VAL  | O-C-CA  | -4.36 | 113.56      | 124.77   |
| 58  | A1    | 102 | FME  | CA-N-CN | 3.80  | 128.67      | 122.82   |
| 58  | A1    | 102 | FME  | C-CA-N  | 3.46  | 116.19      | 109.50   |
| 58  | A1    | 102 | FME  | O-C-CA  | -2.32 | 118.80      | 124.77   |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 58  | A1    | 102 | FME  | N-CA-CB-CG |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

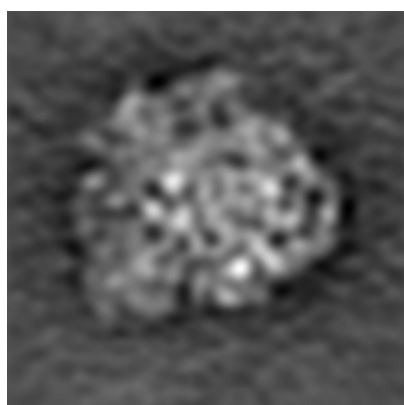
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1717. These allow visual inspection of the internal detail of the map and identification of artifacts.

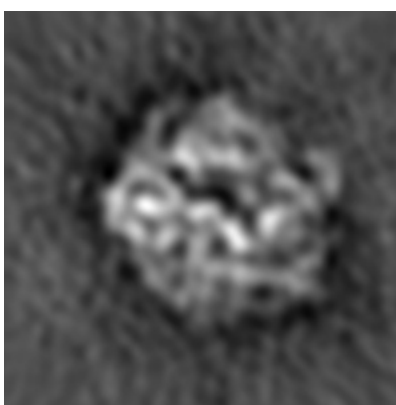
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

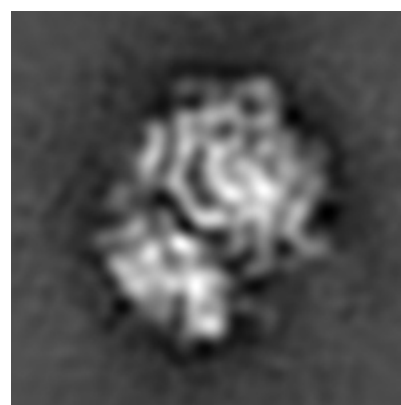
#### 6.1.1 Primary map



X



Y



Z

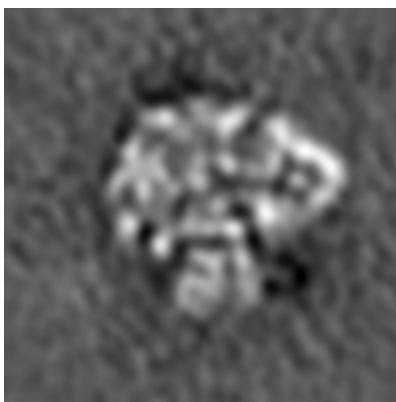
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 64



Y Index: 64



Z Index: 64

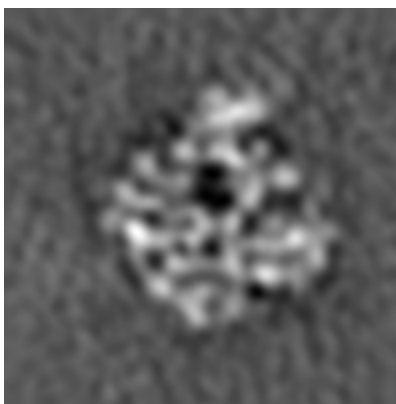
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 65



Y Index: 52

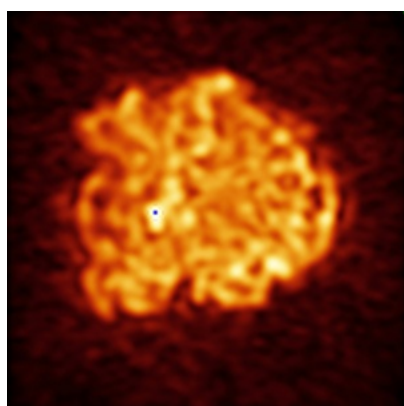


Z Index: 61

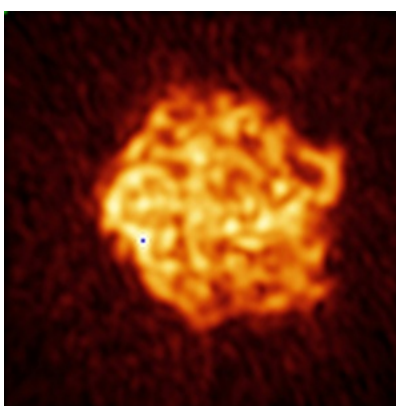
The images above show the largest variance slices of the map in three orthogonal directions.

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

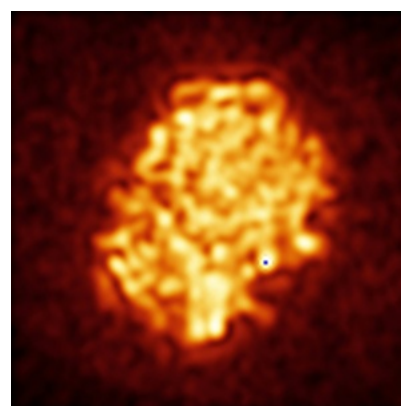
### 6.4.1 Primary map



X



Y

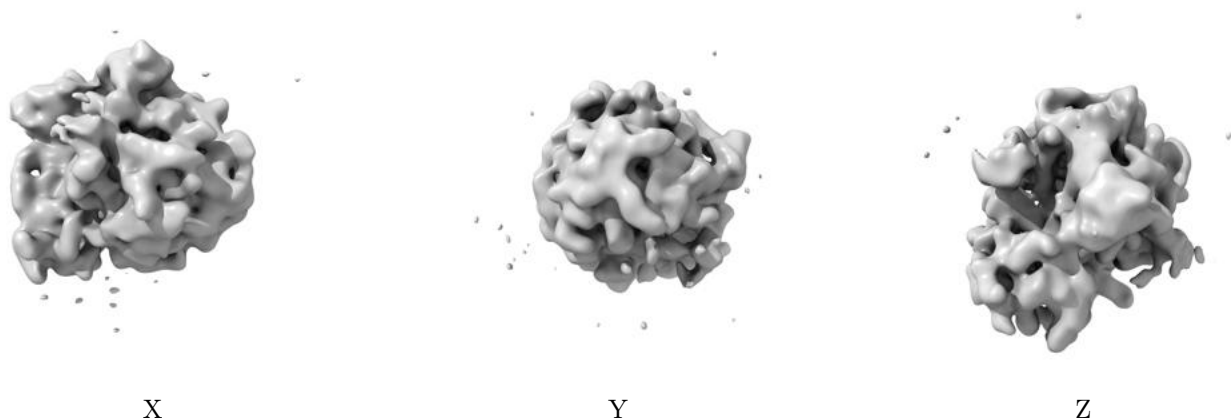


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 22.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

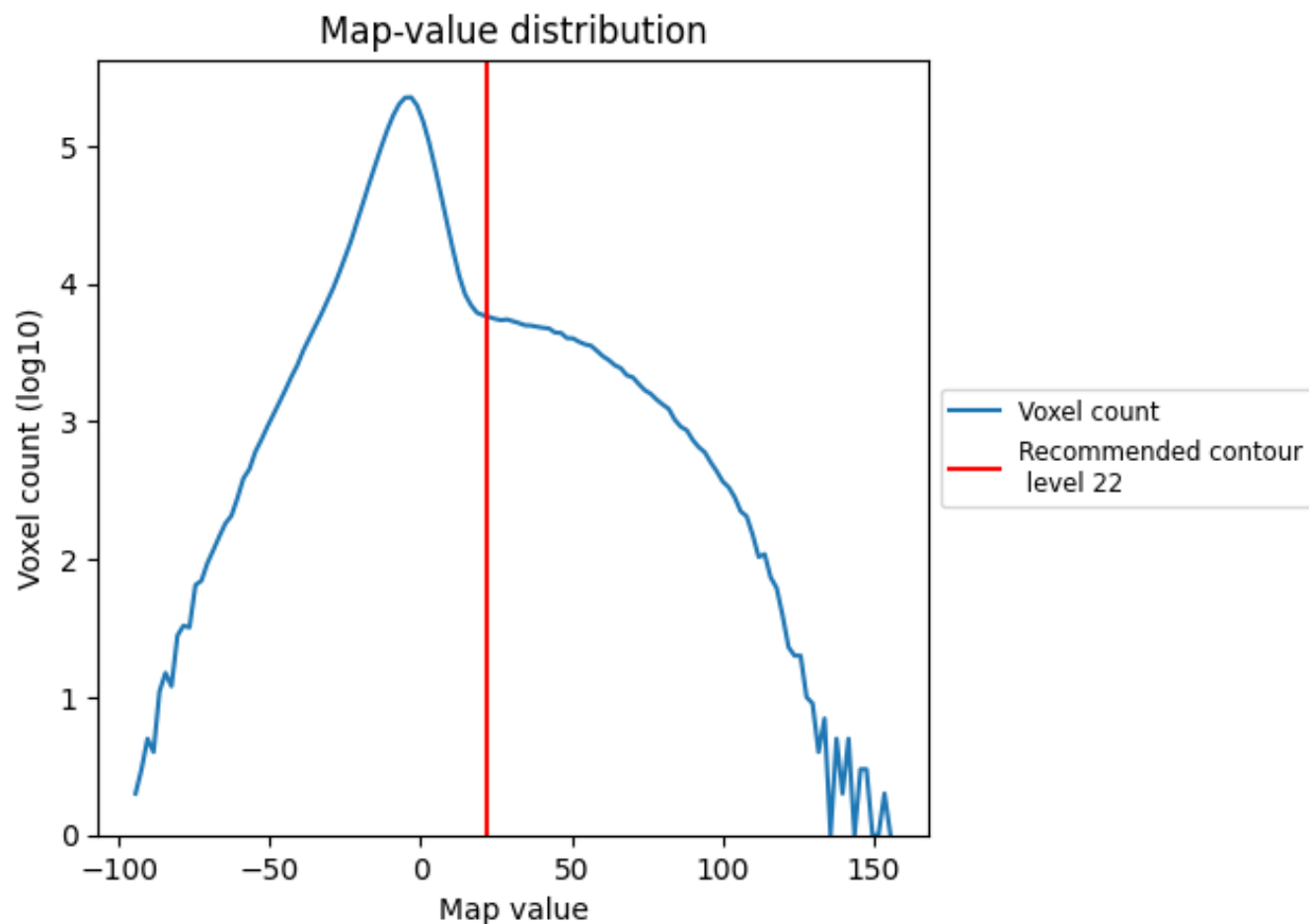
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

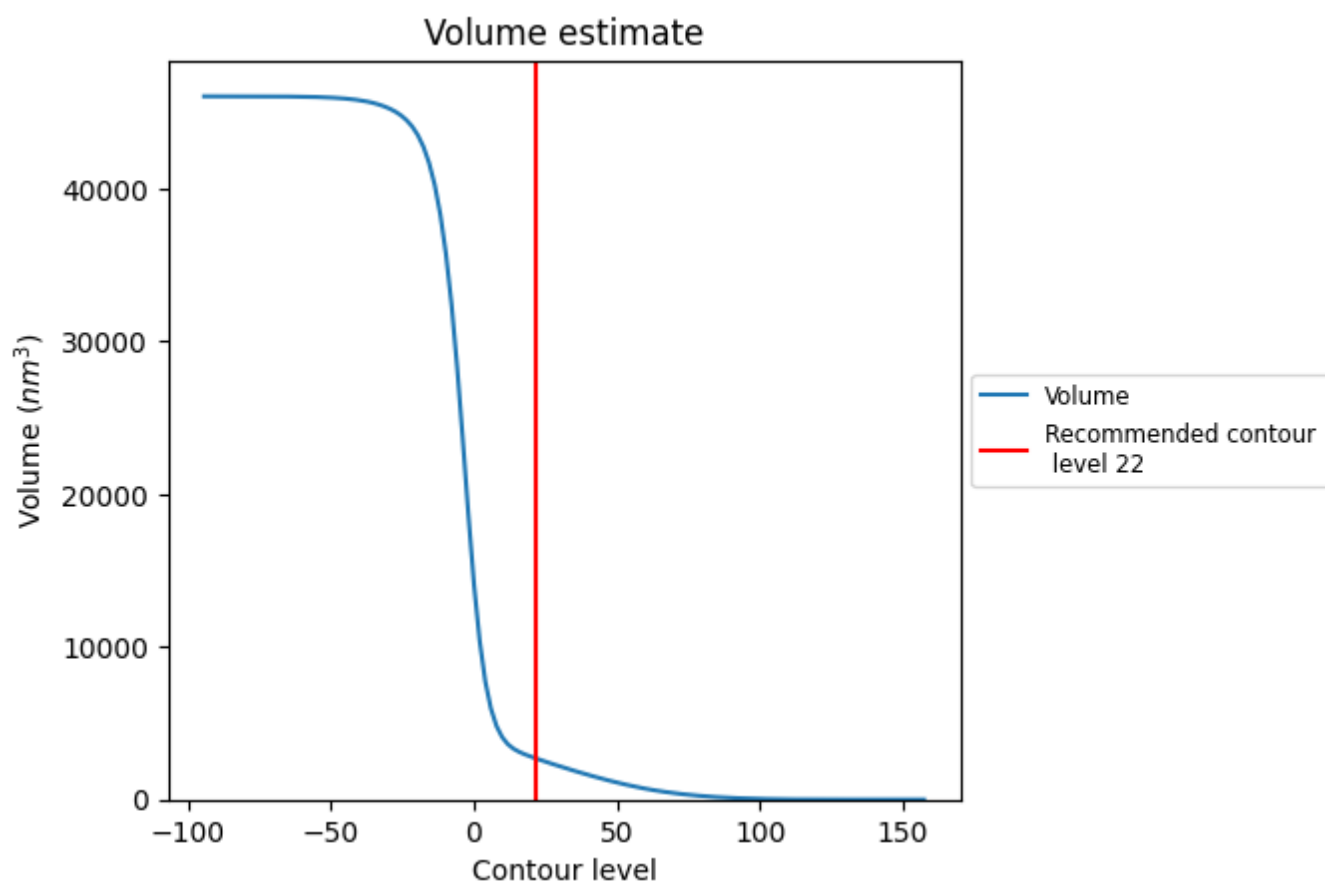
This section contains the results of statistical analysis of the map.

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



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

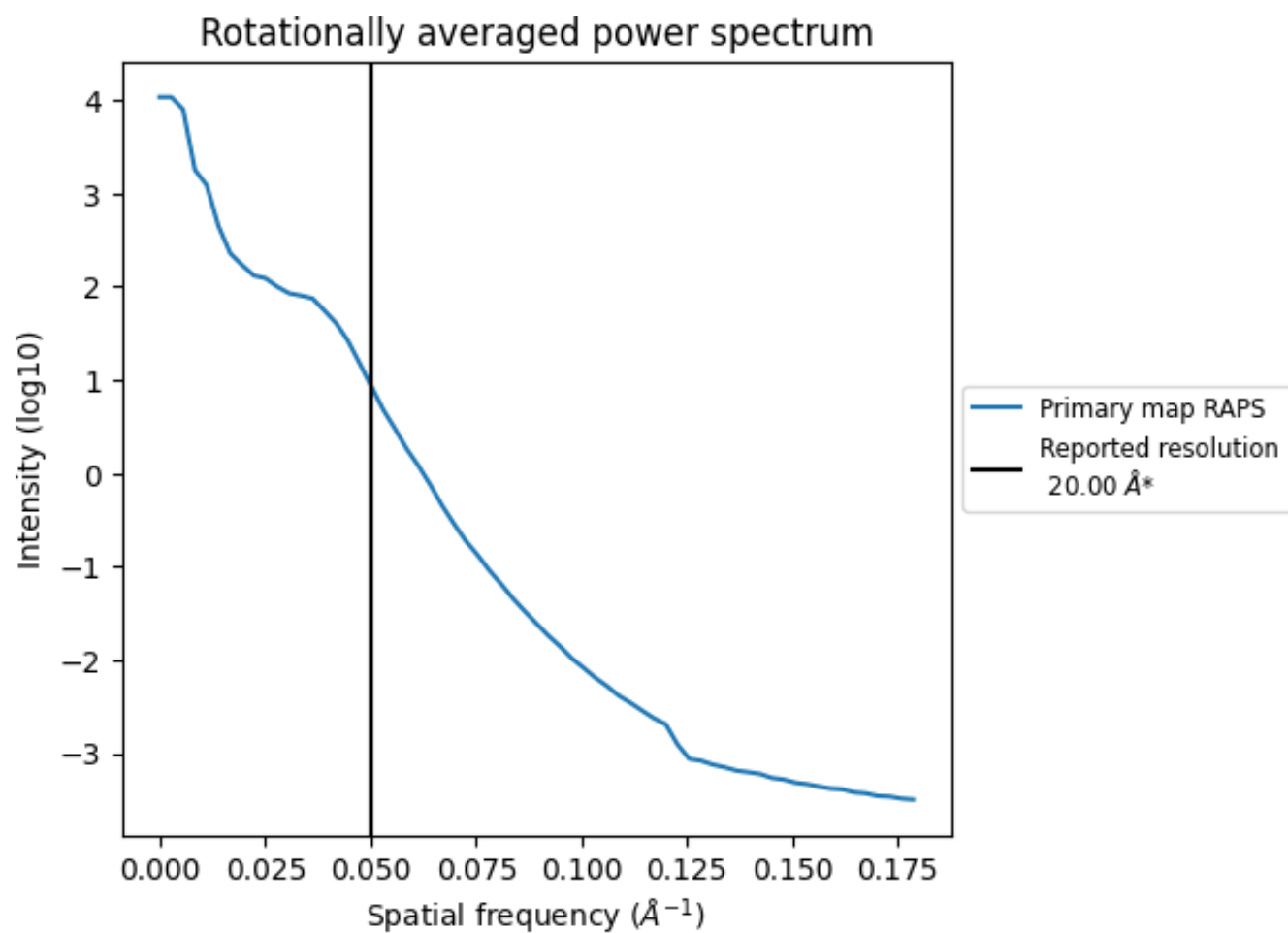
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2675 nm<sup>3</sup>; this corresponds to an approximate mass of 2416 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.050 Å<sup>-1</sup>



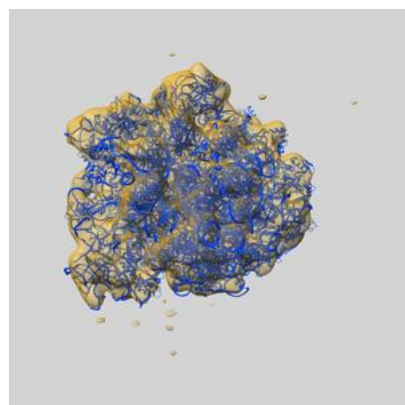
## 8 Fourier-Shell correlation

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

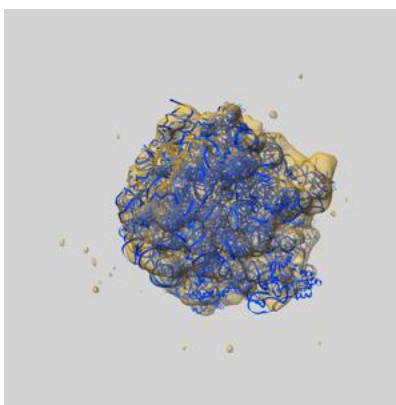
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1717 and PDB model 4V71. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

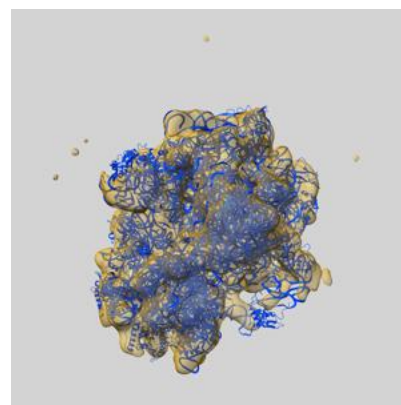
### 9.1 Map-model overlay [i](#)



X



Y



Z

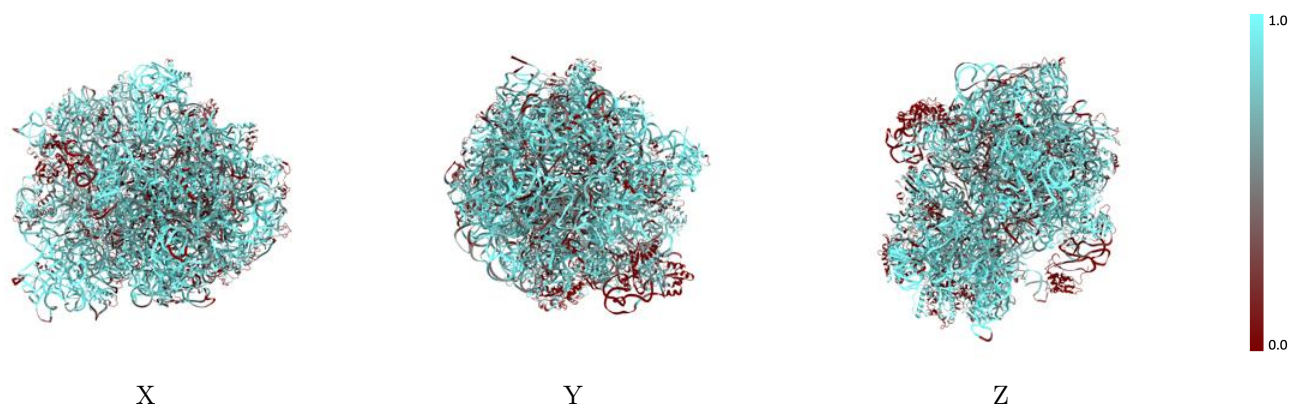
The images above show the 3D surface view of the map at the recommended contour level 22.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



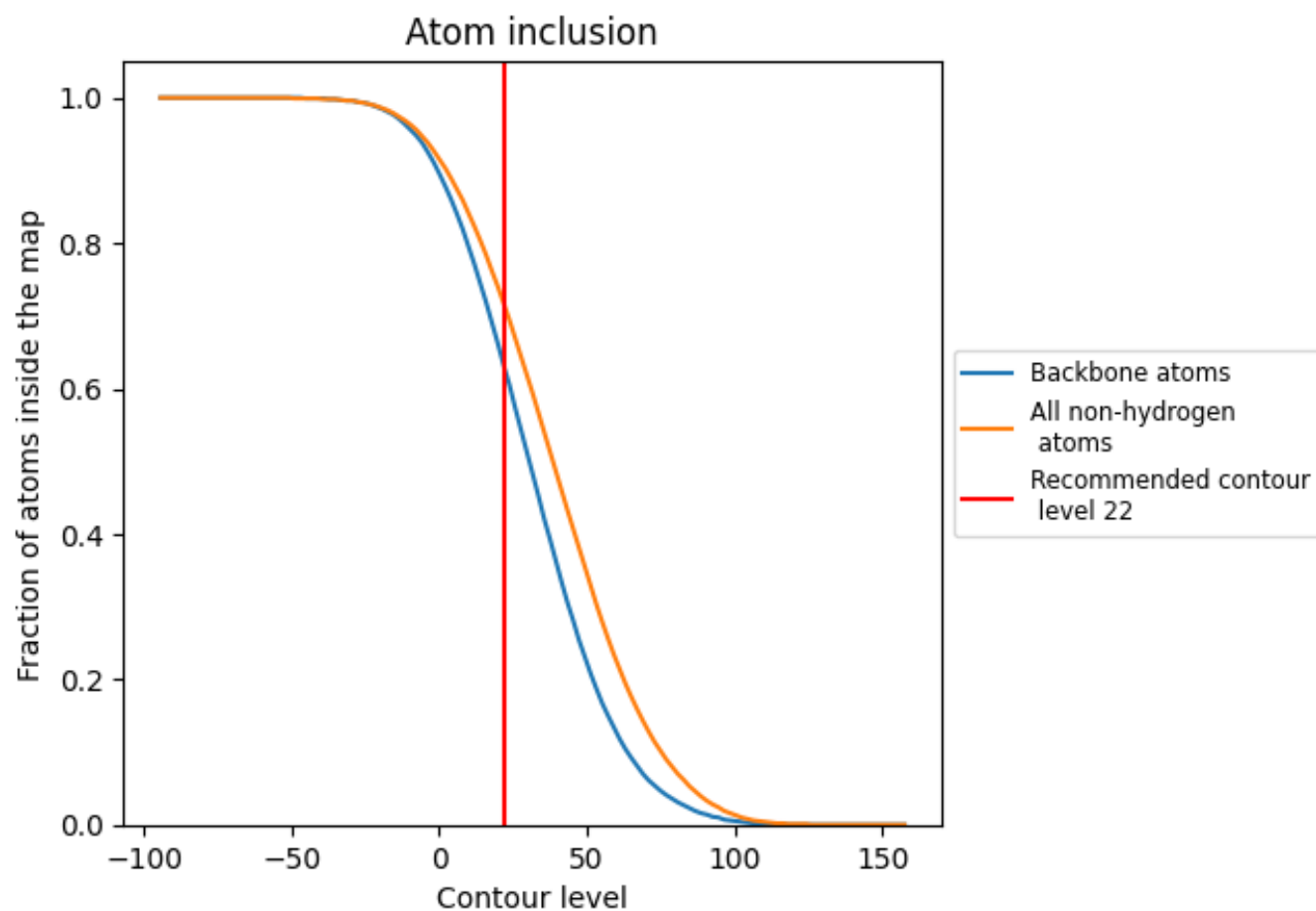
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (22).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 72% 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 (22) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                     |
|-------|--------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| All   |  0.7150   |  0.0490    |
| A1    |  0.5050   |  0.0440    |
| A2    |  0.6080   |  0.0130    |
| A3    |  0.7280   |  0.0490    |
| AA    |  0.8390   |  0.0680    |
| AB    |  0.3960   |  0.0340    |
| AC    |  0.5990   |  0.0420    |
| AD    |  0.4550   |  0.0160    |
| AE    |  0.7970   |  0.0450    |
| AF    |  0.6890   |  0.0520    |
| AG    |  0.4100   |  0.0370    |
| AH    |  0.7610   |  0.0430    |
| AI    |  0.6170   |  0.0220    |
| AJ    |  0.5680   |  0.0070    |
| AK    |  0.5850  |  0.0370   |
| AL    |  0.4920 |  0.0200  |
| AM    |  0.6500 |  0.0540  |
| AN    |  0.6490 |  0.0150  |
| AO    |  0.7120 |  0.0350  |
| AP    |  0.6390 |  0.0420  |
| AQ    |  0.5640 |  0.0150  |
| AR    |  0.5240 |  0.0300  |
| AS    |  0.7150 |  0.0290  |
| AT    |  0.8300 |  0.0310  |
| AU    |  0.4790 |  0.0220  |
| B0    |  0.5650 |  0.0140  |
| B1    |  0.5150 |  0.0330  |
| B2    |  0.3860 |  -0.0040 |
| B3    |  0.5070 |  -0.0550 |
| B4    |  0.8460 |  0.0090  |
| B5    |  0.1850 |  0.0130  |
| BA    |  0.7680 |  0.0570  |
| BB    |  0.8690 |  0.0660  |
| BC    |  0.4290 |  0.0010  |
| BD    |  0.6000 |  0.0030  |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                     |
|-------|--------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| BE    |  0.6330   |  0.0360    |
| BF    |  0.7690   |  0.0510    |
| BG    |  0.6290   |  0.0380    |
| BH    |  0.1310   |  0.0160    |
| BI    |  0.0220   |  0.0170    |
| BJ    |  0.5780   |  0.0020    |
| BK    |  0.4680   |  0.0250    |
| BL    |  0.5210   |  -0.0070   |
| BM    |  0.5700   |  0.0210    |
| BN    |  0.7780   |  0.0210    |
| BO    |  0.8300   |  0.0240    |
| BP    |  0.5920   |  0.0360    |
| BQ    |  0.5930   |  0.0090    |
| BR    |  0.6350   |  0.0420    |
| BS    |  0.5370   |  0.0120    |
| BT    |  0.6820   |  0.0330    |
| BU    |  0.4470   |  0.0190    |
| BV    |  0.7740  |  0.0400   |
| BW    |  0.4980 |  -0.0160 |
| BX    |  0.3250 |  -0.0060 |
| BY    |  0.4570 |  0.0120  |
| BZ    |  0.5680 |  0.0300  |