



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 19, 2016 – 05:21 PM EST

PDB ID : 5MDV  
EMDB ID: : EMD-3489  
Title : Structure of ArfA and RF2 bound to the 70S ribosome (accommodated state)  
Authors : James, N.R.; Brown, A.; Gordiyenko, Y.; Ramakrishnan, V.  
Deposited on : 2016-11-13  
Resolution : 2.97 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

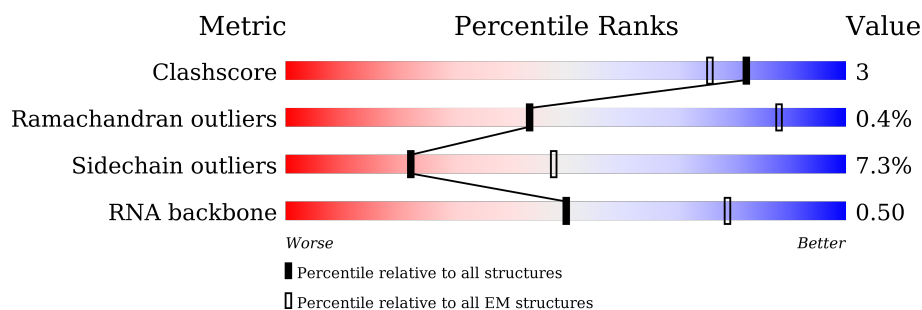
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.97 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.























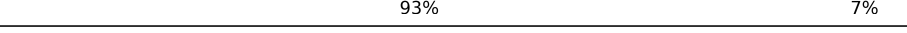




| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 114402                      | 924                         |
| Ramachandran outliers | 111179                      | 726                         |
| Sidechain outliers    | 111093                      | 686                         |
| RNA backbone          | 3027                        | 244                         |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 1     | 2904   | 73% 24% .        |
| 2   | 2     | 1534   | 72% 25% .        |
| 3   | 3     | 120    | 87% 13% .        |
| 4   | 4     | 18     | 22% 6% 72%       |
| 5   | 5     | 78     | 62% 31% 5% .     |
| 6   | 6     | 61     | 57% 18% 25%      |
| 7   | 7     | 365    | 83% 14% ..       |
| 8   | B     | 273    | 86% 12% ..       |

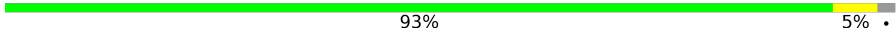

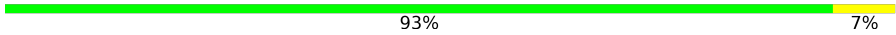
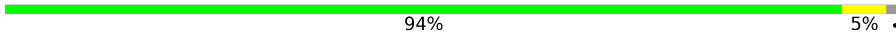



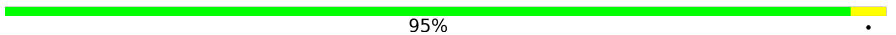



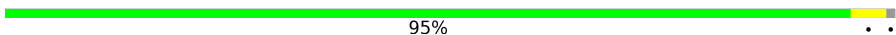





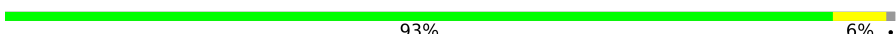

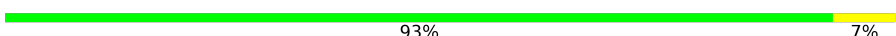




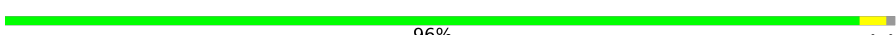
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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 9   | C     | 209    |  89% 11% .     |
| 10  | D     | 201    |  87% 12%       |
| 11  | E     | 179    |  84% 14% ..    |
| 12  | F     | 177    |  89% 9% ..     |
| 13  | G     | 149    |  85% 13% .     |
| 14  | H     | 165    |  61% 16% . 21% |
| 15  | I     | 142    |  79% 15% . 5%  |
| 16  | J     | 142    |  88% 10% .     |
| 17  | K     | 123    |  86% 13% .     |
| 18  | L     | 144    |  83% 15% .     |
| 19  | M     | 136    |  89% 9% .      |
| 20  | N     | 127    |  77% 16% . 6%  |
| 21  | O     | 117    |  81% 17% ..  |
| 22  | P     | 115    |  84% 15% .   |
| 23  | Q     | 118    |  84% 14% ..  |
| 24  | R     | 103    |  92% 8%      |
| 25  | S     | 110    |  79% 20% .   |
| 26  | T     | 100    |  81% 13% 6%  |
| 27  | U     | 104    |  87% 12% ..  |
| 28  | V     | 94     |  93% 7%      |
| 29  | W     | 85     |  82% 7% 11%  |
| 30  | X     | 78     |  81% 18% .   |
| 31  | Y     | 63     |  86% 13% .   |
| 32  | Z     | 59     |  92% 7% .    |
| 33  | a     | 70     |  87% 7% 6%   |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 34  | b     | 57     |  93% 5%      |
| 35  | c     | 55     |  91% 5%      |
| 36  | d     | 46     |  93% 7%      |
| 37  | e     | 65     |  94% 5%      |
| 38  | f     | 38     |  92% 8%      |
| 39  | g     | 241    |  91% 7%      |
| 40  | h     | 233    |  84% 5% 11%  |
| 41  | i     | 206    |  95%         |
| 42  | j     | 167    |  84% 9% 7%   |
| 43  | k     | 135    |  71% 5% 23%  |
| 44  | l     | 179    |  78% 6% 15%  |
| 45  | m     | 130    |  95%        |
| 46  | n     | 130    |  91% 6%    |
| 47  | o     | 103    |  87% 8%    |
| 48  | p     | 129    |  85% 5% 9% |
| 49  | q     | 124    |  92% 7%    |
| 50  | r     | 118    |  90% 8%    |
| 51  | s     | 101    |  93% 6%    |
| 52  | t     | 89     |  87% 12%   |
| 53  | u     | 82     |  93% 7%    |
| 54  | v     | 84     |  90% 5% 5% |
| 55  | w     | 75     |  85% 12%   |
| 56  | x     | 92     |  86% 10%   |
| 57  | y     | 87     |  91% 8%    |
| 58  | z     | 71     |  96%       |

## 2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 149892 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1   | 1     | 2903     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62336 | 27816 | 11470 | 20147 | 2903 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference    |
|-------|---------|----------|--------|----------|--------------|
| 1     | 887     | A        | U      | conflict | GB 802133627 |

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 2   | 2     | 1534     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32929 | 14693 | 6041 | 10661 | 1534 |         |       |

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 3   | 3     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2569  | 1144 | 468 | 837 | 120 |         |       |

- Molecule 4 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 4   | 4     | 5        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 109   | 49 | 22 | 33 | 5 |         |       |

- Molecule 5 is a RNA chain called fMet-NH-tRNA(fMet).

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 5   | 5     | 76       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1622  | 725 | 292 | 528 | 76 | 1 |         |       |

- Molecule 6 is a protein called Alternative ribosome-rescue factor A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | 6     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 234 | 77 | 64 | 2 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| 6     | 0       | HIS      | -      | expression tag | UNP P36675 |

- Molecule 7 is a protein called Peptide chain release factor 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | 7     | 362      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2863  | 1762 | 501 | 590 | 10 |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | B     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | C     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | D     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | E     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | F     | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1313  | 826 | 241 | 244 | 2 |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | G     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | H     | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 980   | 620 | 174 | 182 | 4 |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | I     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 984   | 622 | 171 | 185 | 6 |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | J     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | K     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 946   | 593 | 181 | 166 | 6 |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | L     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | M     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | N     | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 951   | 588 | 195 | 163 | 5 |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 21  | O     | 116      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | P     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 23  | Q     | 117      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | R     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | S     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L23.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | T     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 746   | 470 | 140 | 134 | 2 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | U     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 788   | 498 | 148 | 142 |   |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | V     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | W     | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 582   | 360 | 117 | 104 | 1 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | X     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31  | Y     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 501   | 308 | 98 | 94 | 1 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32  | Z     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 448   | 281 | 87 | 78 | 2 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 33  | a     | 66       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 522   | 323 | 99 | 94 | 6 |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 34  | b     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | c     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 426   | 275 | 78 | 73 |   |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 36  | d     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 37  | e     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L36.

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

- Molecule 39 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39  | g     | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1760  | 1113 | 316 | 323 | 8 |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 40  | h     | 208      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1636  | 1036 | 307 | 290 | 3 |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41  | i     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | j     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 717 | 217 | 212 | 6 |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | k     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 848   | 536 | 153 | 152 | 7 |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | l     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1191  | 741 | 230 | 216 | 4 |         |       |

- Molecule 45 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | m     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 46 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | n     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | o     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 790   | 495 | 151 | 143 | 1 |         |       |

- Molecule 48 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | p     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |       |

- Molecule 49 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | q     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 957   | 591 | 196 | 165 | 5 |         |       |

- Molecule 50 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | r     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 900   | 558 | 181 | 158 | 3 |         |       |

- Molecule 51 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | s     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 52 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | t     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 53 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | u     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 54 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | v     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |       |

- Molecule 55 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 55  | w     | 66       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 544   | 344 | 102 | 97 | 1 |         |       |

- Molecule 56 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | x     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 663   | 424 | 126 | 111 | 2 |         |       |

- Molecule 57 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | y     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 669   | 414 | 138 | 114 | 3 |         |       |

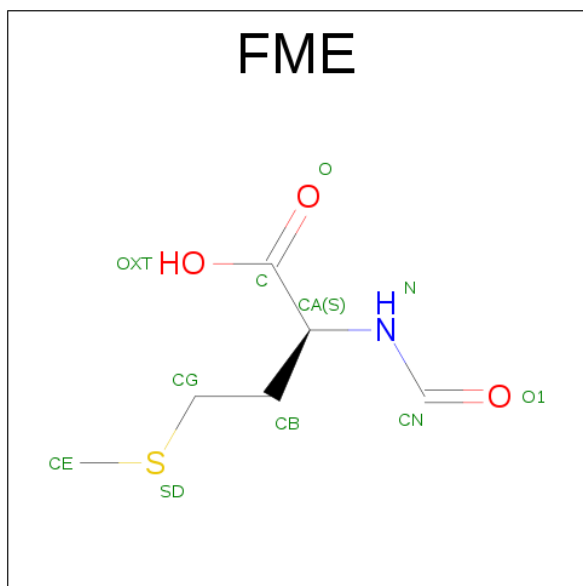
- Molecule 58 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 58  | z     | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 589   | 366 | 125 | 97 | 1 |         |       |

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 59  | 1     | 296      | Total | Mg  | 0       |
|     |       |          | 296   | 296 |         |
| 59  | b     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 59  | i     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 59  | 5     | 4        | Total | Mg  | 0       |
|     |       |          | 4     | 4   |         |
| 59  | 2     | 129      | Total | Mg  | 0       |
|     |       |          | 129   | 129 |         |
| 59  | 3     | 9        | Total | Mg  | 0       |
|     |       |          | 9     | 9   |         |

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula:  $C_6H_{11}NO_3S$ ).



| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 60  | 5     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 10    | 6 | 1 | 2 | 1 |         |

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 61  | a     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 61  | f     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

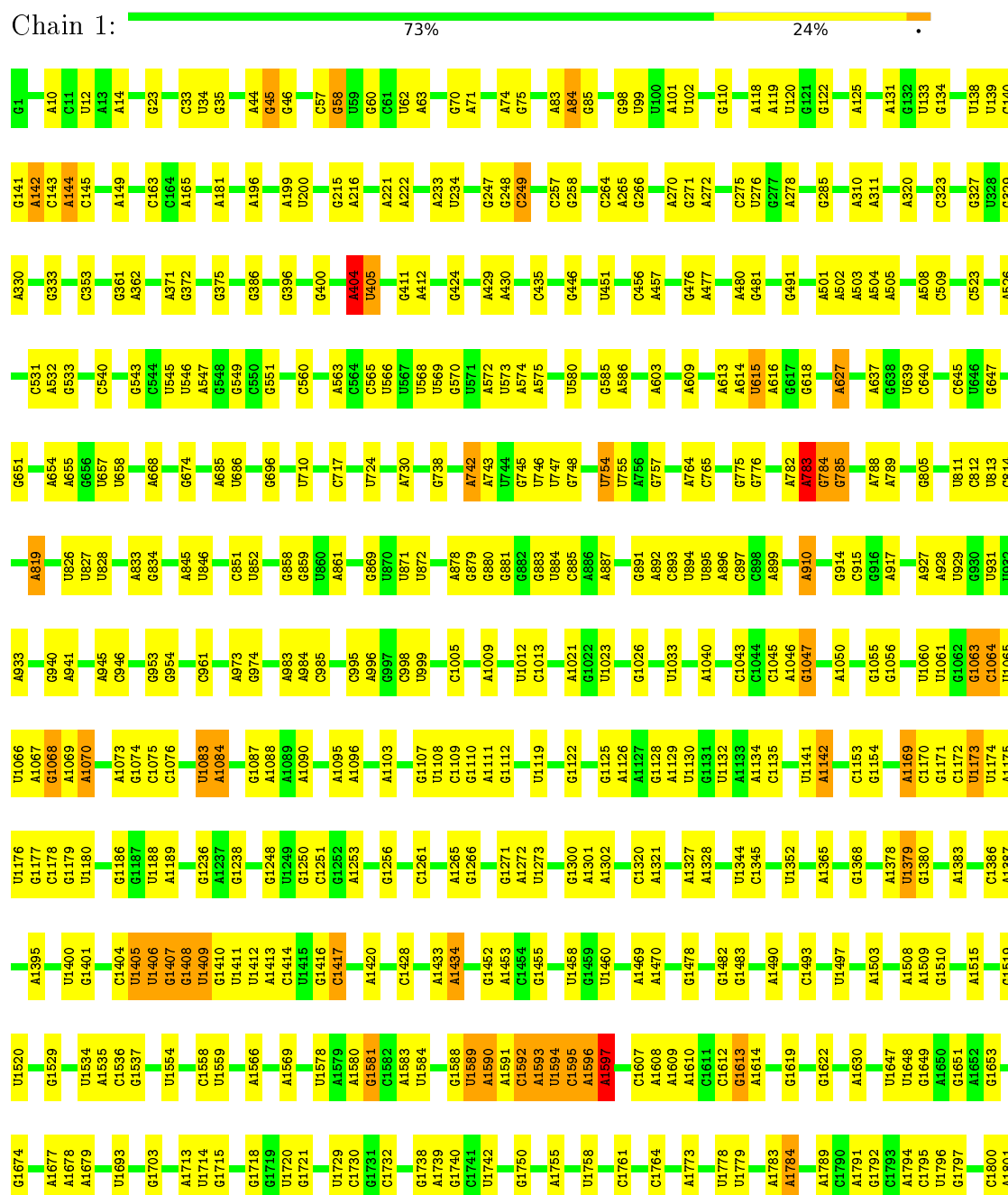
- Molecule 62 is water.

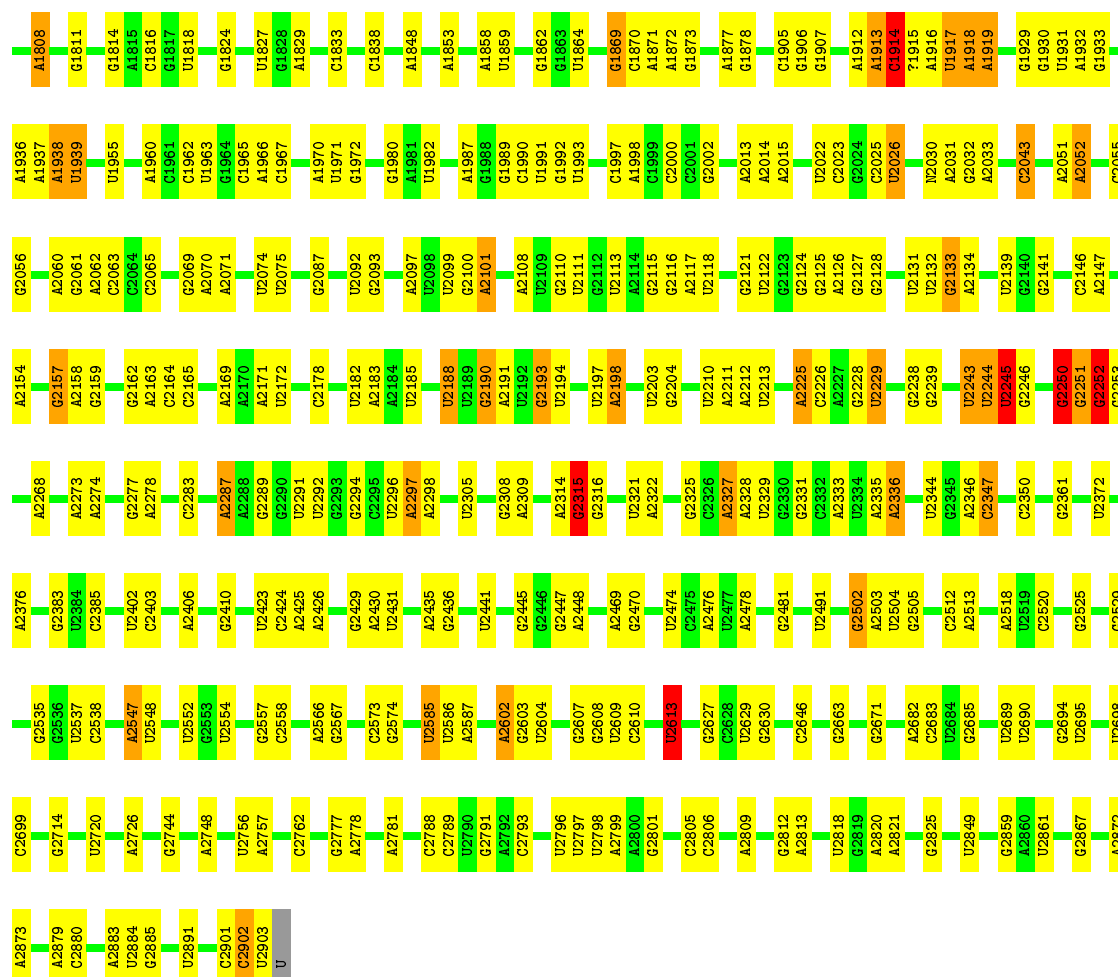
| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 62  | B     | 2        | Total | O | 0       |
|     |       |          | 2     | 2 |         |

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

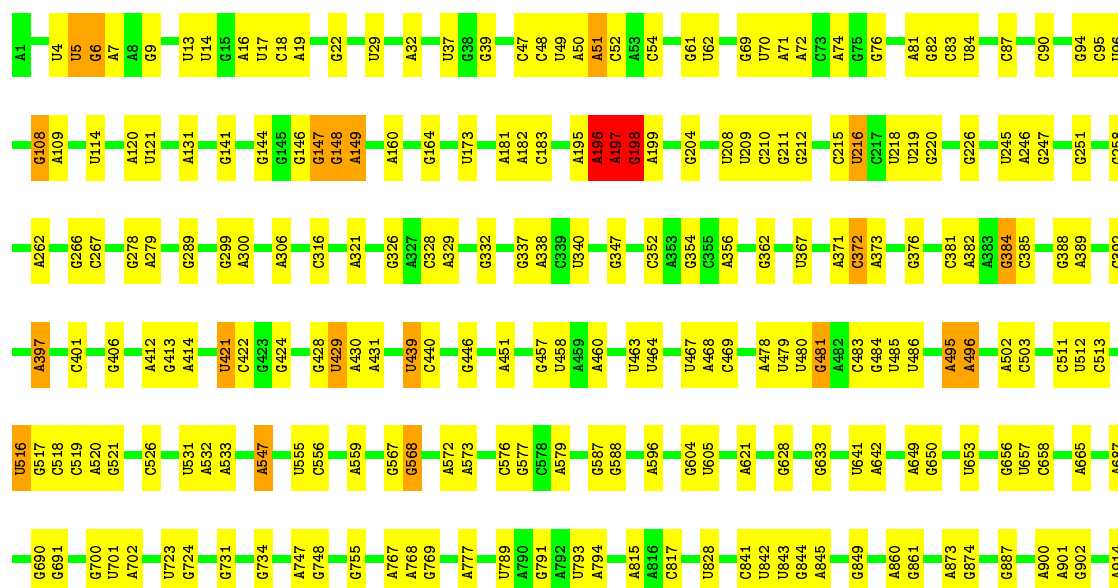
#### • Molecule 1: 23S ribosomal RNA



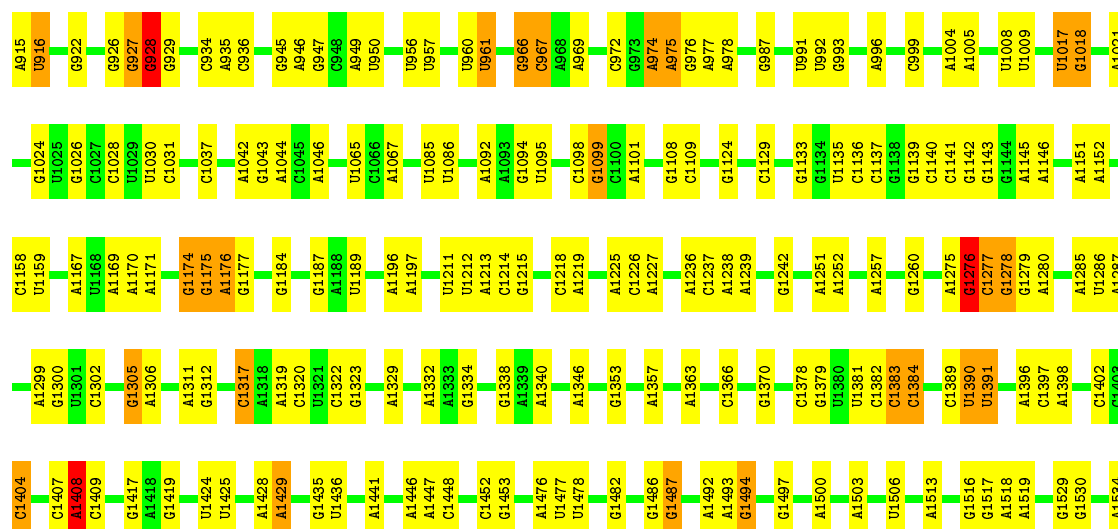


• Molecule 2: 16S ribosomal RNA

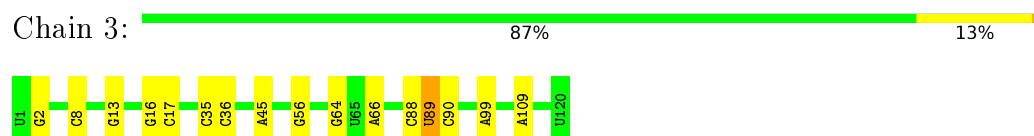
Chain 2: 72% 25%







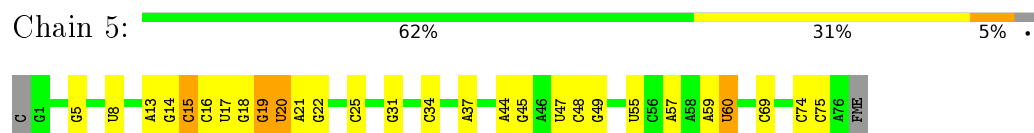
• Molecule 3: 5S ribosomal RNA



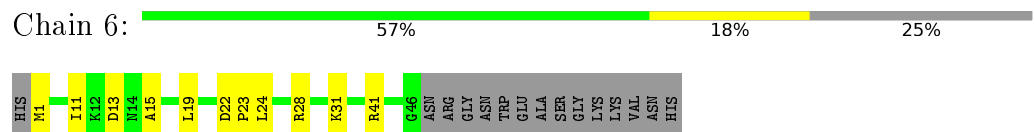
• Molecule 4: mRNA



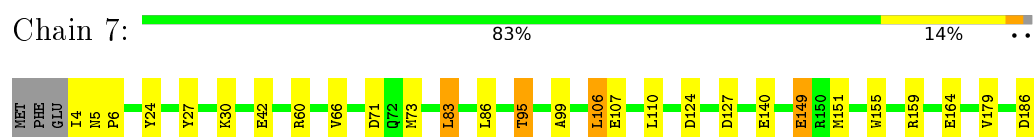
• Molecule 5: fMet-NH-tRNA(fMet)



• Molecule 6: Alternative ribosome-rescue factor A



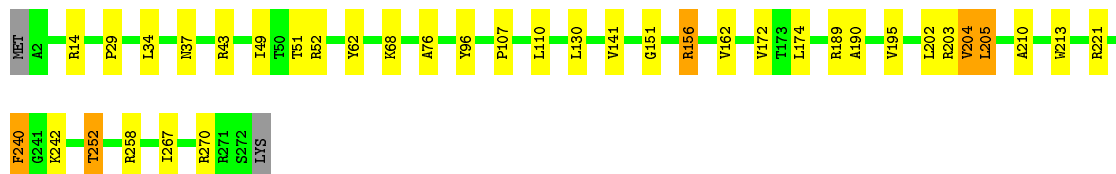
• Molecule 7: Peptide chain release factor 2





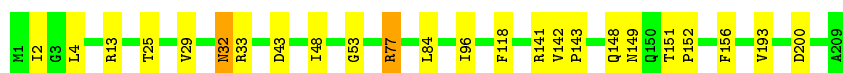
• Molecule 8: 50S ribosomal protein L2

Chain B: 86% 12% ..



• Molecule 9: 50S ribosomal protein L3

Chain C: 89% 11% .



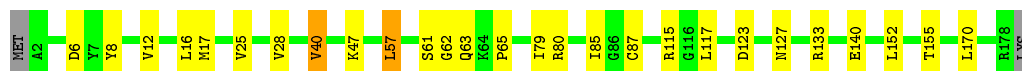
• Molecule 10: 50S ribosomal protein L4

Chain D: 87% 12%



• Molecule 11: 50S ribosomal protein L5

Chain E: 84% 14% ..



• Molecule 12: 50S ribosomal protein L6

Chain F: 89% 9% ..



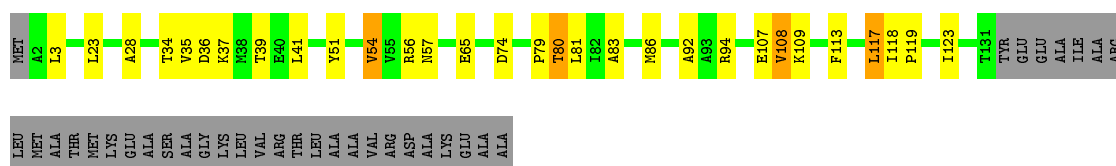
• Molecule 13: 50S ribosomal protein L9

Chain G: 85% 13% .



• Molecule 14: 50S ribosomal protein L10

Chain H: 61% 16% . 21%



- Molecule 15: 50S ribosomal protein L11

Chain I: 79% 15% 5%



- Molecule 16: 50S ribosomal protein L13

Chain J: 88% 10% 2%



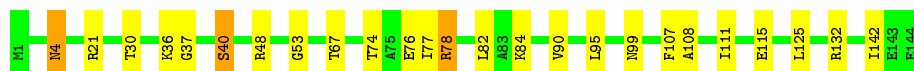
- Molecule 17: 50S ribosomal protein L14

Chain K: 86% 13% 1%



- Molecule 18: 50S ribosomal protein L15

Chain L: 83% 15% 2%



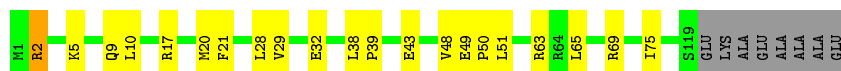
- Molecule 19: 50S ribosomal protein L16

Chain M: 89% 9% 2%



- Molecule 20: 50S ribosomal protein L17

Chain N: 77% 16% 6%



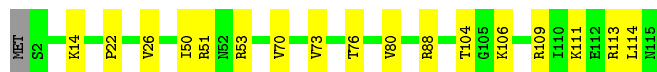
- Molecule 21: 50S ribosomal protein L18

Chain O: 81% 17% 2%



- Molecule 22: 50S ribosomal protein L19

Chain P: 84% 15% .



- Molecule 23: 50S ribosomal protein L20

Chain Q: 84% 14% ..



- Molecule 24: 50S ribosomal protein L21

Chain R: 92% 8%



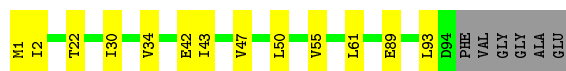
- Molecule 25: 50S ribosomal protein L22

Chain S: 79% 20% .



- Molecule 26: 50S ribosomal protein L23

Chain T: 81% 13% 6%



- Molecule 27: 50S ribosomal protein L24

Chain U: 87% 12% ..

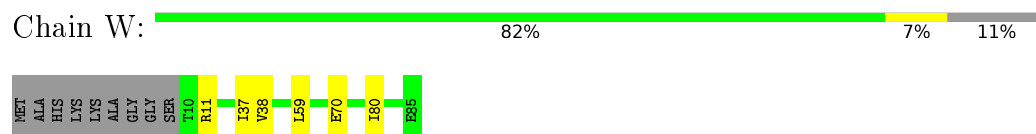


- Molecule 28: 50S ribosomal protein L25

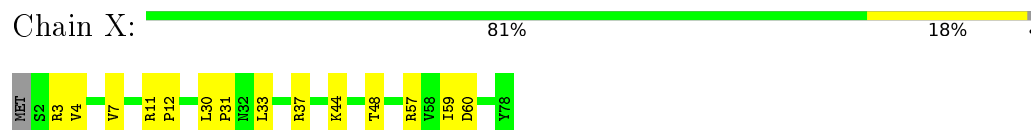
Chain V: 93% 7%



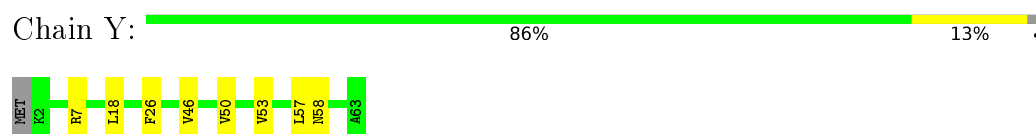
- Molecule 29: 50S ribosomal protein L27



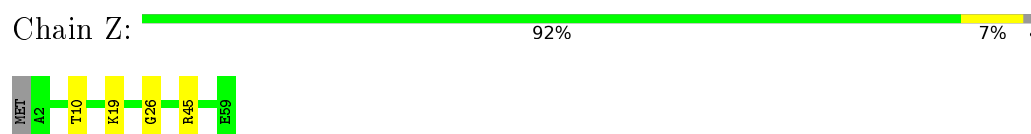
- Molecule 30: 50S ribosomal protein L28



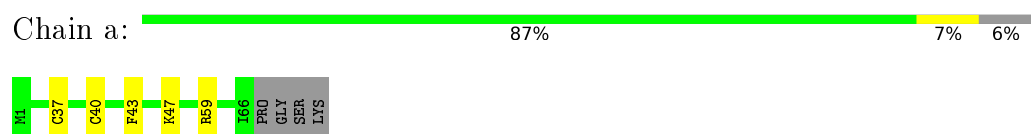
- Molecule 31: 50S ribosomal protein L29



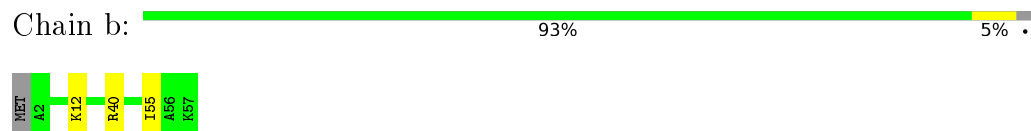
- Molecule 32: 50S ribosomal protein L30



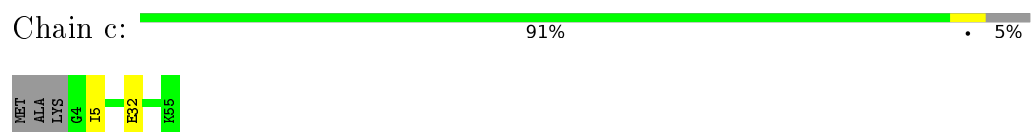
- Molecule 33: 50S ribosomal protein L31



- Molecule 34: 50S ribosomal protein L32



- Molecule 35: 50S ribosomal protein L33



- Molecule 36: 50S ribosomal protein L34





- Molecule 37: 50S ribosomal protein L35

Chain e: 94% 5%



- Molecule 38: 50S ribosomal protein L36

Chain f: 92% 8%



- Molecule 39: 30S ribosomal protein S2

Chain g: 91% 7%



- Molecule 40: 30S ribosomal protein S3

Chain h: 84% 5% 11%



- Molecule 41: 30S ribosomal protein S4

Chain i: 95% 5%



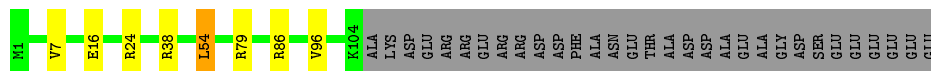
- Molecule 42: 30S ribosomal protein S5

Chain j: 84% 9% 7%

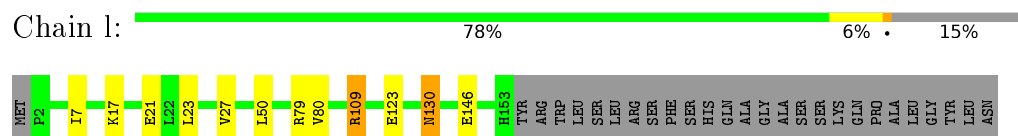


- Molecule 43: 30S ribosomal protein S6

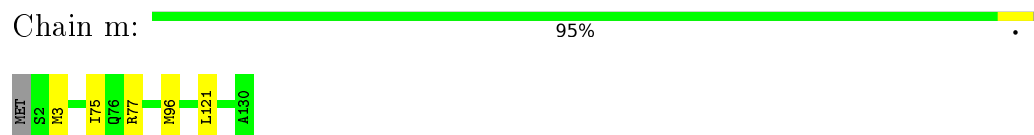
Chain k: 71% 5% 23%



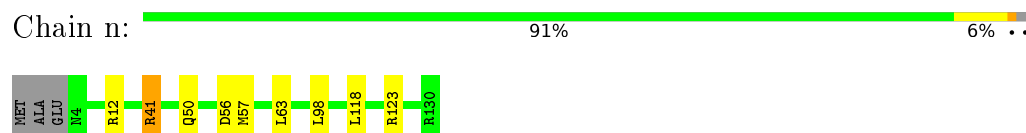
- Molecule 44: 30S ribosomal protein S7



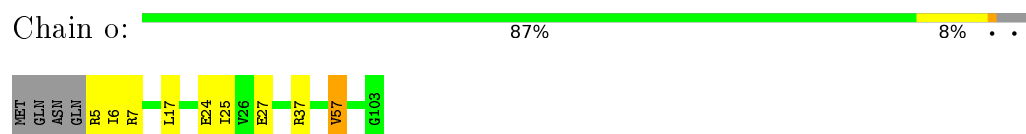
- Molecule 45: 30S ribosomal protein S8



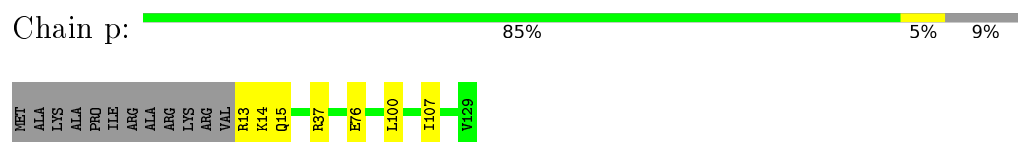
- Molecule 46: 30S ribosomal protein S9



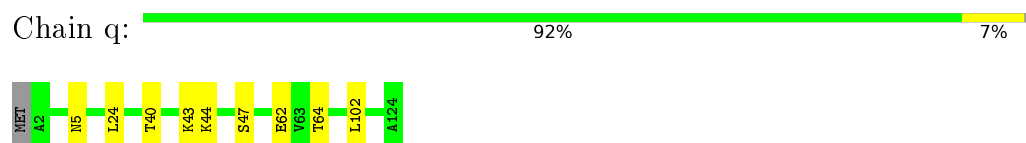
- Molecule 47: 30S ribosomal protein S10



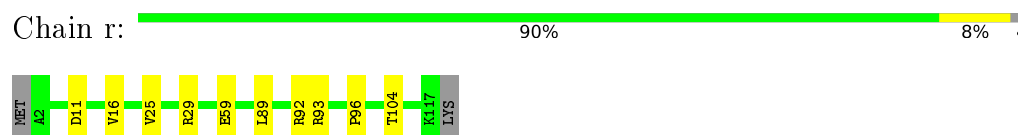
- Molecule 48: 30S ribosomal protein S11



- Molecule 49: 30S ribosomal protein S12



- Molecule 50: 30S ribosomal protein S13




- Molecule 51: 30S ribosomal protein S14

Chain s:  93% 6%



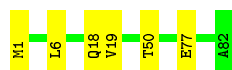
- Molecule 52: 30S ribosomal protein S15

Chain t:  87% 12%



- Molecule 53: 30S ribosomal protein S16

Chain u:  93% 7%



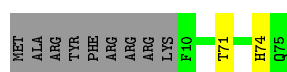
- Molecule 54: 30S ribosomal protein S17

Chain v:  90% 5% 5%




- Molecule 55: 30S ribosomal protein S18

Chain w:  85% 12%



- Molecule 56: 30S ribosomal protein S19

Chain x:  86% 10%



- Molecule 57: 30S ribosomal protein S20

Chain y:  91% 8%



- Molecule 58: 30S ribosomal protein S21

Chain z:  96%





## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, Not provided | Depositor |
| Number of particles used             | 139792              | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF   | Depositor |
| CTF correction method                | Not provided        | Depositor |
| Microscope                           | FEI TITAN KRIOS     | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | Not provided        | Depositor |
| Minimum defocus (nm)                 | 2000                | Depositor |
| Maximum defocus (nm)                 | 3000                | Depositor |
| Magnification                        | 134615              | Depositor |
| Image detector                       | Not provided        | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 0TD, 2MA, 2MG, 1MG, 3TD, G7M, 8AN, UR3, 7MG, 5MU, ZN, OMU, 6MZ, FME, OMC, MG, OMG, H2U, MEQ, 5MC, 4OC, 4SU, PSU

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  >2 | RMSZ        | # Z  >2          |
| 1   | 1     | 0.35         | 0/69286 | 0.72        | 22/108087 (0.0%) |
| 10  | D     | 0.45         | 0/1571  | 0.77        | 1/2113 (0.0%)    |
| 11  | E     | 0.46         | 0/1434  | 0.78        | 0/1926           |
| 12  | F     | 0.39         | 0/1333  | 0.67        | 0/1805           |
| 13  | G     | 0.43         | 0/1122  | 0.67        | 0/1515           |
| 14  | H     | 0.50         | 0/993   | 0.74        | 0/1340           |
| 15  | I     | 0.46         | 0/998   | 0.68        | 0/1348           |
| 16  | J     | 0.44         | 0/1152  | 0.72        | 0/1551           |
| 17  | K     | 0.39         | 0/955   | 0.75        | 0/1279           |
| 18  | L     | 0.43         | 0/1062  | 0.78        | 0/1413           |
| 19  | M     | 0.44         | 0/1093  | 0.78        | 0/1460           |
| 2   | 2     | 0.35         | 0/36590 | 0.73        | 19/57074 (0.0%)  |
| 20  | N     | 0.49         | 0/964   | 0.87        | 0/1289           |
| 21  | O     | 0.47         | 0/902   | 0.80        | 0/1209           |
| 22  | P     | 0.41         | 0/929   | 0.77        | 0/1242           |
| 23  | Q     | 0.57         | 0/960   | 0.89        | 0/1278           |
| 24  | R     | 0.34         | 0/829   | 0.64        | 0/1107           |
| 25  | S     | 0.47         | 0/864   | 0.82        | 0/1156           |
| 26  | T     | 0.41         | 0/752   | 0.72        | 0/1005           |
| 27  | U     | 0.34         | 0/796   | 0.61        | 0/1062           |
| 28  | V     | 0.40         | 0/766   | 0.67        | 0/1025           |
| 29  | W     | 0.42         | 0/589   | 0.75        | 0/779            |
| 3   | 3     | 0.26         | 0/2872  | 0.69        | 0/4478           |
| 30  | X     | 0.46         | 0/635   | 0.80        | 0/848            |
| 31  | Y     | 0.53         | 0/502   | 0.86        | 0/667            |
| 32  | Z     | 0.43         | 0/452   | 0.76        | 0/605            |
| 33  | a     | 0.39         | 0/531   | 0.73        | 0/709            |
| 34  | b     | 0.43         | 0/450   | 0.78        | 0/599            |
| 35  | c     | 0.37         | 0/433   | 0.69        | 0/576            |
| 36  | d     | 0.51         | 0/380   | 0.96        | 0/498            |
| 37  | e     | 0.45         | 0/513   | 0.82        | 0/676            |

| Mol | Chain | Bond lengths |          | Bond angles |                  |
|-----|-------|--------------|----------|-------------|------------------|
|     |       | RMSZ         | # Z  >2  | RMSZ        | # Z  >2          |
| 38  | f     | 0.38         | 0/303    | 0.79        | 0/397            |
| 39  | g     | 0.46         | 0/1791   | 0.70        | 0/2413           |
| 4   | 4     | 0.34         | 0/122    | 0.60        | 0/188            |
| 40  | h     | 0.47         | 0/1663   | 0.74        | 0/2241           |
| 41  | i     | 0.47         | 0/1665   | 0.78        | 0/2227           |
| 42  | j     | 0.50         | 0/1165   | 0.79        | 0/1568           |
| 43  | k     | 0.43         | 0/867    | 0.75        | 1/1171 (0.1%)    |
| 44  | l     | 0.51         | 0/1206   | 0.85        | 1/1617 (0.1%)    |
| 45  | m     | 0.42         | 0/989    | 0.69        | 0/1326           |
| 46  | n     | 0.44         | 0/1034   | 0.81        | 1/1375 (0.1%)    |
| 47  | o     | 0.41         | 0/800    | 0.76        | 0/1082           |
| 48  | p     | 0.41         | 0/893    | 0.74        | 0/1205           |
| 49  | q     | 0.46         | 0/960    | 0.81        | 0/1286           |
| 5   | 5     | 0.29         | 0/1672   | 0.73        | 0/2603           |
| 50  | r     | 0.48         | 0/909    | 0.85        | 0/1215           |
| 51  | s     | 0.50         | 0/817    | 0.80        | 0/1088           |
| 52  | t     | 0.56         | 0/722    | 0.86        | 0/964            |
| 53  | u     | 0.46         | 0/659    | 0.78        | 0/884            |
| 54  | v     | 0.34         | 0/657    | 0.66        | 0/881            |
| 55  | w     | 0.46         | 0/553    | 0.79        | 0/743            |
| 56  | x     | 0.39         | 0/680    | 0.68        | 0/915            |
| 57  | y     | 0.59         | 0/675    | 0.86        | 0/895            |
| 58  | z     | 0.55         | 0/597    | 0.88        | 0/792            |
| 6   | 6     | 0.41         | 0/383    | 0.68        | 0/504            |
| 7   | 7     | 0.49         | 0/2892   | 0.76        | 0/3897           |
| 8   | B     | 0.39         | 0/2121   | 0.78        | 0/2852           |
| 9   | C     | 0.40         | 0/1586   | 0.68        | 0/2134           |
| All | All   | 0.38         | 0/161089 | 0.73        | 45/240182 (0.0%) |

There are no bond length outliers.

All (45) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 2   | 2     | 198  | G    | N9-C1'-C2' | -10.10 | 100.87      | 114.00   |
| 2   | 2     | 1408 | A    | N9-C1'-C2' | -9.66  | 101.38      | 112.00   |
| 2   | 2     | 1404 | C    | N1-C1'-C2' | -9.40  | 101.66      | 112.00   |
| 2   | 2     | 928  | G    | N9-C1'-C2' | -9.08  | 102.01      | 112.00   |
| 2   | 2     | 927  | G    | N9-C1'-C2' | -8.22  | 102.96      | 112.00   |
| 44  | l     | 109  | ARG  | NE-CZ-NH1  | 8.09   | 124.34      | 120.30   |
| 1   | 1     | 2245 | U    | N1-C1'-C2' | -8.00  | 103.19      | 112.00   |
| 1   | 1     | 1914 | C    | N1-C1'-C2' | -7.97  | 103.23      | 112.00   |
| 1   | 1     | 2243 | U    | N1-C1'-C2' | -7.91  | 103.30      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1     | 2193 | G    | C2'-C3'-O3' | 7.17  | 125.26      | 109.50   |
| 1   | 1     | 1597 | A    | N9-C1'-C2'  | -7.14 | 104.14      | 112.00   |
| 1   | 1     | 2252 | G    | N9-C1'-C2'  | -7.03 | 104.27      | 112.00   |
| 1   | 1     | 754  | U    | N1-C1'-C2'  | 6.46  | 122.39      | 114.00   |
| 2   | 2     | 1391 | U    | N1-C1'-C2'  | -6.41 | 104.94      | 112.00   |
| 2   | 2     | 1276 | G    | C1'-C2'-O2' | -6.39 | 91.42       | 110.60   |
| 2   | 2     | 197  | A    | N9-C1'-C2'  | 6.39  | 122.30      | 114.00   |
| 2   | 2     | 927  | G    | C1'-C2'-O2' | -6.26 | 91.82       | 110.60   |
| 1   | 1     | 1379 | U    | C2'-C3'-O3' | 6.24  | 123.69      | 113.70   |
| 1   | 1     | 2244 | U    | C1'-C2'-O2' | -6.20 | 92.01       | 110.60   |
| 1   | 1     | 375  | G    | C2'-C3'-O3' | 6.10  | 123.46      | 113.70   |
| 46  | n     | 41   | ARG  | NE-CZ-NH2   | 5.98  | 123.29      | 120.30   |
| 1   | 1     | 2315 | G    | N9-C1'-C2'  | -5.95 | 105.46      | 112.00   |
| 2   | 2     | 927  | G    | C4'-C3'-O3' | 5.93  | 124.86      | 113.00   |
| 1   | 1     | 2244 | U    | C4'-C3'-O3' | 5.89  | 124.77      | 113.00   |
| 2   | 2     | 1390 | U    | N1-C1'-C2'  | -5.83 | 105.58      | 112.00   |
| 2   | 2     | 1390 | U    | C1'-C2'-O2' | -5.70 | 93.51       | 110.60   |
| 1   | 1     | 742  | A    | C8-N9-C1'   | -5.64 | 117.56      | 127.70   |
| 1   | 1     | 2250 | G    | C4'-C3'-O3' | -5.60 | 97.64       | 109.40   |
| 2   | 2     | 1390 | U    | C4'-C3'-O3' | 5.56  | 124.11      | 113.00   |
| 1   | 1     | 2252 | G    | C4'-C3'-O3' | 5.52  | 124.03      | 113.00   |
| 1   | 1     | 742  | A    | C4-N9-C1'   | 5.47  | 136.15      | 126.30   |
| 1   | 1     | 783  | A    | C4'-C3'-O3' | 5.47  | 123.94      | 113.00   |
| 43  | k     | 54   | LEU  | CA-CB-CG    | 5.47  | 127.87      | 115.30   |
| 2   | 2     | 439  | U    | N1-C1'-C2'  | 5.46  | 121.11      | 114.00   |
| 1   | 1     | 2613 | U    | O4'-C1'-N1  | 5.40  | 112.52      | 108.20   |
| 1   | 1     | 1914 | C    | C4'-C3'-O3' | 5.34  | 123.69      | 113.00   |
| 2   | 2     | 356  | A    | C2'-C3'-O3' | 5.32  | 122.21      | 113.70   |
| 1   | 1     | 742  | A    | N9-C1'-C2'  | 5.31  | 120.90      | 114.00   |
| 2   | 2     | 928  | G    | C4'-C3'-O3' | 5.30  | 123.59      | 113.00   |
| 10  | D     | 69   | ARG  | NE-CZ-NH2   | -5.26 | 117.67      | 120.30   |
| 1   | 1     | 404  | A    | C2'-C3'-O3' | 5.25  | 122.09      | 113.70   |
| 2   | 2     | 1408 | A    | C4'-C3'-O3' | 5.24  | 123.47      | 113.00   |
| 2   | 2     | 1384 | C    | N1-C1'-C2'  | -5.17 | 106.32      | 112.00   |
| 2   | 2     | 196  | A    | N9-C1'-C2'  | -5.10 | 106.39      | 112.00   |
| 1   | 1     | 1838 | C    | N1-C1'-C2'  | 5.03  | 120.54      | 114.00   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 62336 | 0        | 31369    | 269     | 0            |
| 2   | 2     | 32929 | 0        | 16587    | 148     | 0            |
| 3   | 3     | 2569  | 0        | 1301     | 2       | 0            |
| 4   | 4     | 109   | 0        | 55       | 0       | 0            |
| 5   | 5     | 1622  | 0        | 830      | 5       | 0            |
| 6   | 6     | 377   | 0        | 393      | 10      | 0            |
| 7   | 7     | 2863  | 0        | 2760     | 26      | 0            |
| 8   | B     | 2082  | 0        | 2154     | 24      | 0            |
| 9   | C     | 1565  | 0        | 1616     | 16      | 0            |
| 10  | D     | 1552  | 0        | 1619     | 9       | 0            |
| 11  | E     | 1410  | 0        | 1444     | 12      | 0            |
| 12  | F     | 1313  | 0        | 1358     | 9       | 0            |
| 13  | G     | 1111  | 0        | 1148     | 8       | 0            |
| 14  | H     | 980   | 0        | 1013     | 13      | 0            |
| 15  | I     | 984   | 0        | 1035     | 7       | 0            |
| 16  | J     | 1129  | 0        | 1162     | 9       | 0            |
| 17  | K     | 946   | 0        | 1023     | 8       | 0            |
| 18  | L     | 1053  | 0        | 1129     | 13      | 0            |
| 19  | M     | 1074  | 0        | 1157     | 8       | 0            |
| 20  | N     | 951   | 0        | 994      | 11      | 0            |
| 21  | O     | 892   | 0        | 923      | 10      | 0            |
| 22  | P     | 917   | 0        | 962      | 7       | 0            |
| 23  | Q     | 947   | 0        | 1019     | 11      | 0            |
| 24  | R     | 816   | 0        | 839      | 2       | 0            |
| 25  | S     | 857   | 0        | 922      | 13      | 0            |
| 26  | T     | 746   | 0        | 811      | 9       | 0            |
| 27  | U     | 788   | 0        | 843      | 6       | 0            |
| 28  | V     | 753   | 0        | 780      | 1       | 0            |
| 29  | W     | 582   | 0        | 599      | 3       | 0            |
| 30  | X     | 625   | 0        | 652      | 8       | 0            |
| 31  | Y     | 501   | 0        | 531      | 3       | 0            |
| 32  | Z     | 448   | 0        | 488      | 1       | 0            |
| 33  | a     | 522   | 0        | 522      | 0       | 0            |
| 34  | b     | 444   | 0        | 458      | 0       | 0            |
| 35  | c     | 426   | 0        | 464      | 0       | 0            |
| 36  | d     | 377   | 0        | 418      | 0       | 0            |
| 37  | e     | 504   | 0        | 572      | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 38  | f     | 302    | 0        | 341      | 0       | 0            |
| 39  | g     | 1760   | 0        | 1787     | 0       | 0            |
| 40  | h     | 1636   | 0        | 1710     | 0       | 0            |
| 41  | i     | 1643   | 0        | 1707     | 0       | 0            |
| 42  | j     | 1152   | 0        | 1196     | 0       | 0            |
| 43  | k     | 848    | 0        | 846      | 0       | 0            |
| 44  | l     | 1191   | 0        | 1245     | 0       | 0            |
| 45  | m     | 979    | 0        | 1031     | 0       | 0            |
| 46  | n     | 1022   | 0        | 1070     | 0       | 0            |
| 47  | o     | 790    | 0        | 831      | 0       | 0            |
| 48  | p     | 877    | 0        | 887      | 0       | 0            |
| 49  | q     | 957    | 0        | 1017     | 0       | 0            |
| 50  | r     | 900    | 0        | 965      | 0       | 0            |
| 51  | s     | 805    | 0        | 844      | 0       | 0            |
| 52  | t     | 714    | 0        | 734      | 0       | 0            |
| 53  | u     | 649    | 0        | 666      | 0       | 0            |
| 54  | v     | 648    | 0        | 691      | 0       | 0            |
| 55  | w     | 544    | 0        | 560      | 0       | 0            |
| 56  | x     | 663    | 0        | 688      | 0       | 0            |
| 57  | y     | 669    | 0        | 719      | 0       | 0            |
| 58  | z     | 589    | 0        | 629      | 0       | 0            |
| 59  | 1     | 296    | 0        | 0        | 0       | 0            |
| 59  | 2     | 129    | 0        | 0        | 0       | 0            |
| 59  | 3     | 9      | 0        | 0        | 0       | 0            |
| 59  | 5     | 4      | 0        | 0        | 0       | 0            |
| 59  | b     | 1      | 0        | 0        | 0       | 0            |
| 59  | i     | 1      | 0        | 0        | 0       | 0            |
| 60  | 5     | 10     | 0        | 10       | 0       | 0            |
| 61  | a     | 1      | 0        | 0        | 0       | 0            |
| 61  | f     | 1      | 0        | 0        | 0       | 0            |
| 62  | B     | 2      | 0        | 0        | 0       | 0            |
| All | All   | 149892 | 0        | 102124   | 604     | 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 3.

All (604) 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) |
|---------------|---------------|--------------------------|-------------------|
| 2:2:37:U:O4   | 2:2:397:A:N1  | 1.57                     | 1.33              |
| 1:1:2287:A:N1 | 1:1:2344:U:O4 | 1.70                     | 1.24              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1590:A:C2     | 1:1:1591:A:C6     | 2.29                     | 1.19              |
| 1:1:234:U:O4      | 1:1:429:A:N1      | 1.75                     | 1.19              |
| 2:2:148:G:O2'     | 2:2:149:A:C5'     | 1.95                     | 1.15              |
| 1:1:1590:A:C2     | 1:1:1591:A:C5     | 2.40                     | 1.09              |
| 2:2:481:G:O2'     | 2:2:483:C:N4      | 1.85                     | 1.09              |
| 2:2:429:U:N3      | 2:2:431:A:N6      | 2.03                     | 1.07              |
| 1:1:1918:A:O2'    | 1:1:1919:A:N7     | 1.89                     | 1.05              |
| 1:1:1592:C:H2'    | 1:1:1593:A:C8     | 1.97                     | 1.00              |
| 1:1:2013:A:N6     | 1:1:2613:U:H3     | 1.60                     | 0.99              |
| 2:2:148:G:O2'     | 2:2:149:A:O5'     | 1.79                     | 0.99              |
| 2:2:195:A:O2'     | 2:2:196:A:H5'     | 1.61                     | 0.99              |
| 1:1:1406:U:C2'    | 1:1:1407:G:H5''   | 1.93                     | 0.98              |
| 1:1:1405:U:O2'    | 1:1:1406:U:C6     | 2.17                     | 0.97              |
| 1:1:1411:U:H3     | 1:1:1591:A:N6     | 1.64                     | 0.96              |
| 2:2:37:U:H3       | 2:2:397:A:N6      | 1.63                     | 0.96              |
| 1:1:1590:A:N1     | 1:1:1591:A:C6     | 2.32                     | 0.95              |
| 1:1:1590:A:H2'    | 1:1:1591:A:C8     | 2.02                     | 0.94              |
| 1:1:1406:U:H2'    | 1:1:1407:G:H5''   | 1.51                     | 0.92              |
| 2:2:429:U:N3      | 2:2:431:A:C6      | 2.39                     | 0.91              |
| 2:2:148:G:O2'     | 2:2:149:A:H5''    | 1.71                     | 0.91              |
| 1:1:1592:C:H2'    | 1:1:1593:A:H8     | 1.36                     | 0.90              |
| 1:1:1404:C:H2'    | 1:1:1405:U:H5'    | 1.54                     | 0.90              |
| 1:1:2013:A:H61    | 1:1:2613:U:H3     | 1.19                     | 0.89              |
| 1:1:1590:A:N1     | 1:1:1591:A:N6     | 2.19                     | 0.89              |
| 1:1:572:A:OP2     | 24:R:80:ARG:NH2   | 2.06                     | 0.88              |
| 1:1:1411:U:O2     | 1:1:1591:A:N1     | 2.06                     | 0.88              |
| 1:1:1411:U:N3     | 1:1:1591:A:N6     | 2.23                     | 0.86              |
| 1:1:783:A:H2'     | 1:1:783:A:N3      | 1.91                     | 0.85              |
| 2:2:37:U:H3       | 2:2:397:A:H61     | 1.14                     | 0.85              |
| 1:1:1411:U:C2     | 1:1:1591:A:N1     | 2.44                     | 0.85              |
| 2:2:37:U:N3       | 2:2:397:A:N6      | 2.22                     | 0.83              |
| 12:F:121:ILE:HD12 | 12:F:141:ILE:HG22 | 1.61                     | 0.82              |
| 2:2:439:U:O2      | 2:2:440:C:C6      | 2.33                     | 0.82              |
| 2:2:13:U:O4       | 2:2:915:A:N6      | 2.12                     | 0.82              |
| 1:1:1404:C:C2'    | 1:1:1405:U:H5'    | 2.10                     | 0.81              |
| 1:1:2315:G:O2'    | 1:1:2316:G:O4'    | 1.98                     | 0.81              |
| 2:2:481:G:HO2'    | 2:2:483:C:N4      | 1.75                     | 0.81              |
| 2:2:1277:C:O2'    | 2:2:1278:G:P      | 2.39                     | 0.81              |
| 2:2:37:U:C4       | 2:2:397:A:N1      | 2.49                     | 0.80              |
| 2:2:429:U:C4      | 2:2:431:A:N6      | 2.49                     | 0.80              |
| 2:2:1277:C:O2'    | 2:2:1278:G:O5'    | 2.00                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1779:U:H5     | 1:1:1784:A:N7     | 1.80                     | 0.79              |
| 1:1:234:U:N3      | 1:1:429:A:N6      | 2.31                     | 0.78              |
| 1:1:1596:A:O2'    | 1:1:1597:A:C5'    | 2.33                     | 0.77              |
| 9:C:4:LEU:HD23    | 9:C:29:VAL:HG11   | 1.66                     | 0.76              |
| 1:1:1405:U:O2'    | 1:1:1406:U:O4'    | 2.03                     | 0.75              |
| 14:H:36:ASP:O     | 14:H:39:THR:OG1   | 2.05                     | 0.75              |
| 2:2:197:A:O2'     | 2:2:220:G:N2      | 2.20                     | 0.75              |
| 1:1:1047:G:HO2'   | 1:1:1110:G:H1     | 1.36                     | 0.74              |
| 1:1:1084:A:N7     | 14:H:37:LYS:NZ    | 2.35                     | 0.74              |
| 2:2:195:A:C2'     | 2:2:196:A:H5'     | 2.18                     | 0.74              |
| 1:1:1595:C:O2'    | 1:1:1596:A:H5'    | 1.88                     | 0.73              |
| 1:1:1596:A:O2'    | 1:1:1597:A:H5'    | 1.88                     | 0.73              |
| 1:1:927:A:H2'     | 1:1:928:A:C8      | 2.23                     | 0.73              |
| 2:2:37:U:O4       | 2:2:397:A:C2      | 2.42                     | 0.72              |
| 1:1:1607:C:N4     | 1:1:1622:G:OP2    | 2.23                     | 0.71              |
| 7:7:83:LEU:HD21   | 7:7:95:THR:HG22   | 1.72                     | 0.71              |
| 2:2:148:G:O2'     | 2:2:149:A:P       | 2.48                     | 0.71              |
| 2:2:1277:C:HO2'   | 2:2:1278:G:P      | 2.12                     | 0.70              |
| 1:1:1590:A:N3     | 1:1:1591:A:C5     | 2.59                     | 0.70              |
| 1:1:2315:G:O2'    | 1:1:2316:G:O5'    | 2.09                     | 0.70              |
| 1:1:234:U:C4      | 1:1:429:A:N1      | 2.58                     | 0.70              |
| 1:1:568:U:H1'     | 1:1:2030:6MZ:H9C1 | 1.73                     | 0.69              |
| 1:1:2013:A:N6     | 1:1:2613:U:N3     | 2.29                     | 0.69              |
| 1:1:585:G:N7      | 23:Q:6:ARG:NH1    | 2.40                     | 0.69              |
| 1:1:1824:G:O2'    | 8:B:252:THR:HG21  | 1.92                     | 0.69              |
| 1:1:2287:A:N1     | 1:1:2344:U:C4     | 2.59                     | 0.69              |
| 29:W:59:LEU:HD12  | 29:W:80:ILE:HD12  | 1.75                     | 0.69              |
| 1:1:742:A:H2'     | 1:1:743:A:C8      | 2.29                     | 0.68              |
| 21:O:27:VAL:HG21  | 21:O:40:ILE:HD12  | 1.76                     | 0.67              |
| 1:1:2065:C:H4'    | 1:1:2251:OMG:CM2  | 2.24                     | 0.67              |
| 1:1:1411:U:O2     | 1:1:1591:A:C2     | 2.48                     | 0.67              |
| 1:1:754:U:H2'     | 1:1:755:U:C6      | 2.30                     | 0.67              |
| 8:B:162:VAL:HG11  | 8:B:174:LEU:HD12  | 1.77                     | 0.66              |
| 15:I:78:LEU:HD22  | 15:I:108:ILE:HG23 | 1.77                     | 0.66              |
| 1:1:1913:A:C2     | 2:2:1492:A:O2'    | 2.47                     | 0.66              |
| 2:2:429:U:C2      | 2:2:431:A:N6      | 2.63                     | 0.66              |
| 10:D:108:ILE:HD11 | 10:D:180:LEU:HD13 | 1.77                     | 0.66              |
| 2:2:769:G:H4'     | 2:2:1513:A:H4'    | 1.76                     | 0.65              |
| 8:B:29:PRO:HG2    | 8:B:34:LEU:HD11   | 1.76                     | 0.65              |
| 1:1:1590:A:O2'    | 1:1:1591:A:O4'    | 2.13                     | 0.65              |
| 12:F:35:ARG:HD3   | 12:F:71:LEU:HD13  | 1.79                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:2000:C:OP1   | 20:N:5:LYS:NZ     | 2.29                     | 0.65              |
| 25:S:36:LEU:HD13 | 25:S:48:LYS:HA    | 1.79                     | 0.64              |
| 1:1:2065:C:H4'   | 1:1:2251:OMG:HM22 | 1.79                     | 0.64              |
| 2:2:1277:C:O2'   | 2:2:1278:G:C5'    | 2.46                     | 0.64              |
| 1:1:1913:A:H2    | 2:2:1492:A:HO2'   | 1.40                     | 0.64              |
| 1:1:1916:A:H2'   | 1:1:1917:PSU:C6   | 2.33                     | 0.64              |
| 1:1:1405:U:O2'   | 1:1:1406:U:H6     | 1.77                     | 0.63              |
| 1:1:84:A:N1      | 1:1:98:G:O2'      | 2.30                     | 0.63              |
| 2:2:148:G:HO2'   | 2:2:149:A:C5'     | 2.11                     | 0.63              |
| 8:B:141:VAL:HG11 | 8:B:190:ALA:HB1   | 1.81                     | 0.63              |
| 1:1:1653:G:H3'   | 20:N:2:ARG:HG2    | 1.79                     | 0.62              |
| 10:D:48:THR:HG23 | 10:D:86:ALA:HB3   | 1.81                     | 0.62              |
| 11:E:57:LEU:HD12 | 11:E:87:CYS:SG    | 2.39                     | 0.62              |
| 1:1:1590:A:C2    | 1:1:1591:A:C4     | 2.88                     | 0.61              |
| 2:2:658:C:H1'    | 26:T:22:THR:HG21  | 118.50                   | 0.61              |
| 28:V:75:GLN:HB2  | 28:V:92:VAL:HG23  | 1.83                     | 0.61              |
| 7:7:194:THR:O    | 7:7:337:ARG:NH2   | 2.33                     | 0.61              |
| 1:1:929:U:H1'    | 32:Z:26:GLY:O     | 2.00                     | 0.61              |
| 1:1:1405:U:C2'   | 1:1:1406:U:C6     | 2.82                     | 0.61              |
| 1:1:1590:A:H2'   | 1:1:1591:A:H8     | 1.63                     | 0.60              |
| 1:1:1153:C:OP1   | 23:Q:92:ARG:NH1   | 2.33                     | 0.60              |
| 21:O:31:THR:O    | 21:O:102:ARG:NH1  | 2.33                     | 0.60              |
| 1:1:1998:A:OP2   | 9:C:141:ARG:NH2   | 2.34                     | 0.60              |
| 1:1:1779:U:C5    | 1:1:1784:A:N7     | 2.68                     | 0.60              |
| 2:2:928:G:O2'    | 2:2:929:G:C5'     | 2.50                     | 0.60              |
| 8:B:76:ALA:HB2   | 8:B:96:TYR:CD1    | 2.37                     | 0.60              |
| 1:1:1913:A:H2    | 2:2:1492:A:O2'    | 1.85                     | 0.59              |
| 1:1:2683:C:O2    | 17:K:70:ARG:NH2   | 2.35                     | 0.59              |
| 2:2:1518:MA6:N6  | 2:2:1519:MA6:H93  | 2.17                     | 0.59              |
| 31:Y:18:LEU:HB2  | 31:Y:53:VAL:HG11  | 1.84                     | 0.59              |
| 10:D:104:ALA:O   | 10:D:108:ILE:HG23 | 2.02                     | 0.59              |
| 27:U:34:VAL:HG13 | 27:U:67:VAL:HG22  | 1.85                     | 0.59              |
| 8:B:107:PRO:HD2  | 8:B:110:LEU:HD22  | 1.84                     | 0.59              |
| 1:1:2627:G:O2'   | 1:1:2781:A:N1     | 2.33                     | 0.59              |
| 2:2:13:U:C4      | 2:2:915:A:N6      | 2.68                     | 0.58              |
| 7:7:268:THR:HG21 | 7:7:298:LEU:CD2   | 2.33                     | 0.58              |
| 18:L:76:GLU:HB2  | 18:L:111:ILE:HD11 | 1.84                     | 0.58              |
| 1:1:1063:G:O2'   | 1:1:1064:C:O4'    | 2.21                     | 0.58              |
| 1:1:2289:G:N2    | 1:1:2344:U:O2     | 2.35                     | 0.58              |
| 2:2:146:G:O2'    | 2:2:147:G:H5'     | 2.03                     | 0.58              |
| 2:2:148:G:O2'    | 2:2:149:A:C4'     | 2.52                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:2720:U:OP1    | 22:P:53:ARG:NH2   | 2.37                     | 0.58              |
| 10:D:130:LYS:HB2  | 10:D:133:LEU:HD12 | 1.85                     | 0.58              |
| 1:1:1411:U:C4     | 1:1:1591:A:N6     | 2.61                     | 0.58              |
| 1:1:1095:A:H2'    | 1:1:1096:A:C8     | 2.39                     | 0.58              |
| 1:1:1410:G:O6     | 1:1:1592:C:N3     | 2.36                     | 0.58              |
| 16:J:28:LEU:HD12  | 16:J:142:ILE:HG22 | 1.86                     | 0.58              |
| 1:1:1915:3TD:O2   | 2:2:1409:C:H4'    | 2.04                     | 0.57              |
| 1:1:1590:A:C2     | 1:1:1591:A:N1     | 2.69                     | 0.57              |
| 1:1:1937:A:O2'    | 1:1:1939:5MU:H71  | 2.03                     | 0.57              |
| 1:1:2245:U:O2'    | 1:1:2436:G:OP2    | 2.23                     | 0.57              |
| 1:1:1592:C:C2'    | 1:1:1593:A:C8     | 2.82                     | 0.57              |
| 18:L:37:GLY:H     | 18:L:40:SER:HB3   | 1.68                     | 0.57              |
| 2:2:1218:C:H2'    | 2:2:1219:A:C8     | 2.40                     | 0.57              |
| 2:2:14:U:OP2      | 6:6:41:ARG:NH2    | 2.38                     | 0.57              |
| 18:L:82:LEU:HD22  | 18:L:90:VAL:HG21  | 1.87                     | 0.57              |
| 1:1:1789:A:OP2    | 8:B:221:ARG:NH1   | 2.38                     | 0.56              |
| 1:1:1938:A:H5'    | 1:1:1939:5MU:H71  | 1.86                     | 0.56              |
| 2:2:37:U:O2       | 2:2:547:A:H2      | 1.88                     | 0.56              |
| 1:1:1596:A:O2'    | 1:1:1597:A:O4'    | 2.23                     | 0.56              |
| 2:2:1174:G:H2'    | 2:2:1175:G:H5'    | 1.86                     | 0.56              |
| 1:1:1411:U:N3     | 1:1:1591:A:C6     | 2.65                     | 0.56              |
| 2:2:198:G:H2'     | 2:2:199:A:H8      | 1.70                     | 0.56              |
| 30:X:12:PRO:HB3   | 30:X:30:LEU:HD23  | 1.88                     | 0.56              |
| 1:1:2683:C:OP1    | 22:P:51:ARG:NH2   | 2.37                     | 0.56              |
| 2:2:1382:C:C2'    | 2:2:1383:C:H5'    | 2.36                     | 0.56              |
| 15:I:105:LEU:HD13 | 15:I:129:GLU:HG2  | 1.86                     | 0.56              |
| 2:2:1169:A:H2'    | 2:2:1170:A:C8     | 2.41                     | 0.56              |
| 17:K:41:ILE:HD11  | 17:K:86:LEU:HD22  | 1.88                     | 0.56              |
| 13:G:72:ILE:HD11  | 13:G:108:VAL:HA   | 1.87                     | 0.56              |
| 7:7:249:ALA:CB    | 7:7:254:VAL:HG11  | 2.36                     | 0.55              |
| 1:1:2315:G:O2'    | 1:1:2316:G:C5'    | 2.53                     | 0.55              |
| 25:S:74:ILE:HD12  | 25:S:105:VAL:HG22 | 1.88                     | 0.55              |
| 1:1:1406:U:O2'    | 1:1:1407:G:H5''   | 2.07                     | 0.55              |
| 17:K:113:MET:O    | 17:K:116:ILE:HG13 | 2.07                     | 0.55              |
| 2:2:496:A:N3      | 2:2:496:A:H2'     | 2.21                     | 0.55              |
| 13:G:96:THR:HG22  | 13:G:117:LEU:HD12 | 1.88                     | 0.55              |
| 1:1:1405:U:H2'    | 1:1:1406:U:C6     | 2.42                     | 0.55              |
| 1:1:1261:C:OP2    | 25:S:83:LYS:NZ    | 2.41                     | 0.54              |
| 2:2:1109:C:O4'    | 2:2:1109:C:C5'    | 2.55                     | 0.54              |
| 2:2:148:G:HO2'    | 2:2:149:A:C4'     | 2.19                     | 0.54              |
| 20:N:10:LEU:HD11  | 20:N:43:GLU:HG3   | 1.88                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:2252:G:H2'   | 1:1:2253:G:H8     | 1.71                     | 0.54              |
| 1:1:2502:G:H5''  | 1:1:2503:2MA:H5'' | 1.89                     | 0.54              |
| 2:2:146:G:C2'    | 2:2:147:G:H5'     | 2.36                     | 0.54              |
| 6:6:24:LEU:O     | 6:6:28:ARG:NH2    | 2.40                     | 0.54              |
| 29:W:37:ILE:HG21 | 29:W:80:ILE:HG21  | 1.90                     | 0.54              |
| 1:1:2315:G:O2'   | 1:1:2316:G:H8     | 1.89                     | 0.54              |
| 11:E:8:TYR:HA    | 11:E:12:VAL:HB    | 1.89                     | 0.54              |
| 30:X:3:ARG:HD2   | 30:X:30:LEU:HD22  | 1.89                     | 0.54              |
| 14:H:23:LEU:HD13 | 14:H:92:ALA:HA    | 1.90                     | 0.54              |
| 1:1:1141:U:H4'   | 1:1:1142:A:O4'    | 2.08                     | 0.54              |
| 1:1:811:U:H2'    | 18:L:21:ARG:HA    | 1.90                     | 0.54              |
| 1:1:1916:A:H2'   | 1:1:1917:PSU:H6   | 1.73                     | 0.54              |
| 2:2:439:U:H2'    | 2:2:439:U:O2      | 2.08                     | 0.53              |
| 1:1:1980:G:O2'   | 1:1:1982:U:OP2    | 2.25                     | 0.53              |
| 1:1:742:A:C2     | 1:1:743:A:C6      | 2.97                     | 0.53              |
| 2:2:429:U:O2     | 2:2:430:A:N7      | 2.40                     | 0.53              |
| 1:1:1590:A:C6    | 1:1:1591:A:N6     | 2.76                     | 0.53              |
| 1:1:783:A:H8     | 1:1:1778:U:O2'    | 1.90                     | 0.53              |
| 21:O:99:TYR:OH   | 21:O:111:ARG:NH1  | 2.41                     | 0.53              |
| 1:1:2685:G:OP1   | 17:K:78:ARG:NH2   | 2.42                     | 0.53              |
| 1:1:1614:A:C2    | 25:S:93:ALA:HB2   | 2.44                     | 0.53              |
| 20:N:29:VAL:HG11 | 20:N:75:ILE:HG23  | 1.91                     | 0.53              |
| 19:M:66:ARG:NH1  | 19:M:104:GLU:OE1  | 2.35                     | 0.53              |
| 1:1:2901:C:H2'   | 1:1:2902:C:C6     | 2.44                     | 0.53              |
| 1:1:404:A:O2'    | 1:1:405:U:OP2     | 2.22                     | 0.53              |
| 1:1:2244:U:H2'   | 1:1:2245:U:C6     | 2.44                     | 0.53              |
| 2:2:431:A:O5'    | 2:2:431:A:H8      | 1.92                     | 0.53              |
| 2:2:371:A:H2'    | 2:2:372:C:O4'     | 2.09                     | 0.52              |
| 1:1:234:U:H3     | 1:1:429:A:N6      | 2.06                     | 0.52              |
| 1:1:783:A:N3     | 1:1:783:A:C2'     | 2.70                     | 0.52              |
| 1:1:2902:C:C2'   | 1:1:2903:U:H5'    | 2.40                     | 0.52              |
| 2:2:1277:C:O2'   | 2:2:1278:G:H5''   | 2.08                     | 0.52              |
| 2:2:5:U:O4'      | 2:2:5:U:O2        | 2.27                     | 0.52              |
| 1:1:2805:C:H2'   | 1:1:2806:C:O4'    | 2.08                     | 0.52              |
| 8:B:76:ALA:HB2   | 8:B:96:TYR:CE1    | 2.44                     | 0.52              |
| 1:1:320:A:H2'    | 10:D:131:THR:HG21 | 1.91                     | 0.52              |
| 1:1:639:U:H2'    | 1:1:640:C:C6      | 2.45                     | 0.52              |
| 1:1:674:G:O2'    | 10:D:69:ARG:HD3   | 2.09                     | 0.52              |
| 2:2:246:A:N1     | 2:2:278:G:O2'     | 2.39                     | 0.52              |
| 2:2:429:U:O2     | 2:2:430:A:C8      | 2.62                     | 0.52              |
| 1:1:1915:3TD:H2' | 1:1:1916:A:C8     | 2.45                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:2243:U:H2'   | 1:1:2244:U:C6    | 2.45                     | 0.52              |
| 2:2:1277:C:HO2'  | 2:2:1278:G:C5'   | 2.21                     | 0.52              |
| 1:1:1913:A:C6    | 2:2:1494:G:C8    | 2.98                     | 0.52              |
| 2:2:928:G:O2'    | 2:2:929:G:O4'    | 2.26                     | 0.52              |
| 1:1:2346:A:H4'   | 1:1:2347:C:OP2   | 2.09                     | 0.52              |
| 9:C:152:PRO:HG3  | 9:C:156:PHE:CZ   | 2.45                     | 0.52              |
| 2:2:966:2MG:H2'  | 2:2:966:2MG:N3   | 2.24                     | 0.52              |
| 1:1:1915:3TD:H4' | 6:6:13:ASP:HB2   | 1.92                     | 0.52              |
| 7:7:73:MET:SD    | 7:7:110:LEU:HB2  | 2.49                     | 0.52              |
| 1:1:2250:G:OP1   | 19:M:84:LYS:NZ   | 2.27                     | 0.51              |
| 7:7:73:MET:SD    | 7:7:106:LEU:HD12 | 2.51                     | 0.51              |
| 1:1:1869:G:N2    | 1:1:1871:A:O2'   | 2.44                     | 0.51              |
| 1:1:954:G:OP2    | 19:M:16:ARG:NH2  | 2.44                     | 0.51              |
| 26:T:50:LEU:HD23 | 31:Y:26:PHE:CZ   | 2.45                     | 0.51              |
| 1:1:2287:A:C2    | 1:1:2344:U:O4    | 2.58                     | 0.51              |
| 1:1:1250:G:OP2   | 18:L:21:ARG:NH2  | 2.43                     | 0.51              |
| 1:1:1405:U:H2'   | 1:1:1406:U:C5    | 2.45                     | 0.51              |
| 1:1:1939:5MU:OP1 | 1:1:2604:U:O2'   | 2.28                     | 0.51              |
| 7:7:24:TYR:CG    | 7:7:362:LYS:HB3  | 2.46                     | 0.51              |
| 1:1:2331:G:O2'   | 1:1:2336:A:N1    | 2.35                     | 0.51              |
| 1:1:2287:A:N6    | 1:1:2344:U:H3    | 2.09                     | 0.51              |
| 2:2:966:2MG:HM22 | 5:5:34:C:H5"     | 1.93                     | 0.51              |
| 1:1:570:G:H2'    | 1:1:2030:6MZ:N7  | 2.26                     | 0.51              |
| 2:2:928:G:O2'    | 2:2:929:G:H5'    | 2.10                     | 0.51              |
| 1:1:1056:G:O2'   | 1:1:1103:A:N6    | 2.44                     | 0.51              |
| 1:1:2469:A:N6    | 1:1:2481:G:O2'   | 2.44                     | 0.51              |
| 2:2:555:U:H2'    | 2:2:556:C:C6     | 2.46                     | 0.51              |
| 7:7:281:HIS:ND1  | 19:M:78:LEU:HD23 | 2.26                     | 0.50              |
| 6:6:24:LEU:HD11  | 7:7:319:TRP:CE3  | 2.46                     | 0.50              |
| 7:7:151:MET:SD   | 7:7:353:LEU:HD21 | 2.51                     | 0.50              |
| 3:3:8:C:O3'      | 21:O:25:ARG:NH1  | 2.44                     | 0.50              |
| 1:1:2287:A:N6    | 1:1:2344:U:N3    | 2.59                     | 0.50              |
| 15:I:38:CYS:SG   | 15:I:39:LYS:N    | 2.85                     | 0.50              |
| 16:J:35:ARG:HB3  | 16:J:54:ILE:HD11 | 1.93                     | 0.50              |
| 21:O:27:VAL:CG2  | 21:O:40:ILE:HD12 | 2.41                     | 0.50              |
| 2:2:1424:U:H2'   | 2:2:1425:U:O4'   | 2.12                     | 0.50              |
| 2:2:1383:C:H2'   | 2:2:1384:C:C6    | 2.47                     | 0.50              |
| 20:N:49:GLU:HB2  | 20:N:50:PRO:HD3  | 1.93                     | 0.50              |
| 1:1:580:U:O3'    | 23:Q:31:VAL:HG13 | 2.10                     | 0.50              |
| 6:6:11:ILE:HG21  | 6:6:15:ALA:HA    | 1.94                     | 0.50              |
| 1:1:1590:A:N3    | 1:1:1591:A:C4    | 2.80                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:2052:A:H4'   | 9:C:148:GLN:O     | 2.12                     | 0.50              |
| 1:1:1591:A:H2'   | 1:1:1592:C:C6     | 2.47                     | 0.49              |
| 1:1:1818:U:OP2   | 8:B:156:ARG:NH1   | 2.46                     | 0.49              |
| 2:2:198:G:H2'    | 2:2:199:A:C8      | 2.46                     | 0.49              |
| 2:2:966:2MG:H5'' | 2:2:967:5MC:OP2   | 2.13                     | 0.49              |
| 1:1:998:C:OP2    | 23:Q:58:ARG:NH2   | 2.45                     | 0.49              |
| 1:1:1932:A:H2'   | 1:1:1933:G:O4'    | 2.12                     | 0.49              |
| 1:1:2093:G:O2'   | 1:1:2198:A:N1     | 2.41                     | 0.49              |
| 2:2:519:C:H2'    | 2:2:520:A:O4'     | 2.13                     | 0.49              |
| 5:5:44:A:H2'     | 5:5:45:G:O4'      | 2.13                     | 0.49              |
| 7:7:253:HIS:O    | 7:7:256:ARG:HG3   | 2.13                     | 0.49              |
| 7:7:24:TYR:CD2   | 7:7:362:LYS:HB3   | 2.47                     | 0.49              |
| 8:B:141:VAL:CG1  | 8:B:190:ALA:HB1   | 2.42                     | 0.49              |
| 1:1:1154:G:OP2   | 23:Q:58:ARG:NH1   | 2.44                     | 0.49              |
| 9:C:4:LEU:HD23   | 9:C:29:VAL:CG1    | 2.40                     | 0.49              |
| 18:L:132:ARG:HG3 | 18:L:142:ILE:HD12 | 1.93                     | 0.49              |
| 1:1:2297:A:N1    | 1:1:2321:U:C5     | 2.81                     | 0.49              |
| 1:1:2585:U:O2    | 1:1:2585:U:O4'    | 2.30                     | 0.49              |
| 13:G:99:ILE:O    | 13:G:103:VAL:HG23 | 2.13                     | 0.49              |
| 18:L:4:ASN:C     | 18:L:4:ASN:HD22   | 2.15                     | 0.49              |
| 1:1:871:U:H2'    | 1:1:872:U:C6      | 2.48                     | 0.49              |
| 2:2:1225:A:H2'   | 2:2:1226:C:C5     | 2.48                     | 0.49              |
| 1:1:1693:U:O2'   | 8:B:14:ARG:NH2    | 2.45                     | 0.49              |
| 17:K:38:ILE:HD11 | 17:K:112:PHE:CZ   | 2.48                     | 0.49              |
| 1:1:2291:U:H2'   | 1:1:2292:U:C6     | 2.47                     | 0.49              |
| 1:1:783:A:C8     | 1:1:1778:U:O2'    | 2.66                     | 0.49              |
| 2:2:1305:G:HO2'  | 2:2:1306:A:H8     | 1.55                     | 0.49              |
| 16:J:30:THR:HG22 | 16:J:31:GLU:N     | 2.28                     | 0.49              |
| 14:H:118:ILE:HB  | 14:H:119:PRO:HD3  | 1.94                     | 0.48              |
| 7:7:5:ASN:N      | 7:7:6:PRO:CD      | 2.76                     | 0.48              |
| 1:1:1408:G:H2'   | 1:1:1409:U:C6     | 2.48                     | 0.48              |
| 2:2:1383:C:H2'   | 2:2:1384:C:H6     | 1.78                     | 0.48              |
| 2:2:502:A:H2'    | 2:2:503:C:O4'     | 2.13                     | 0.48              |
| 1:1:1792:G:H5'   | 8:B:204:VAL:HG23  | 1.95                     | 0.48              |
| 12:F:24:ILE:CD1  | 12:F:72:LEU:HD21  | 2.43                     | 0.48              |
| 1:1:1084:A:OP1   | 14:H:54:VAL:HG12  | 2.13                     | 0.48              |
| 7:7:281:HIS:CE1  | 19:M:78:LEU:HD23  | 2.48                     | 0.48              |
| 9:C:33:ARG:NH1   | 9:C:53:GLY:O      | 2.42                     | 0.48              |
| 14:H:23:LEU:HD12 | 14:H:118:ILE:HG21 | 1.96                     | 0.48              |
| 20:N:38:LEU:N    | 20:N:39:PRO:CD    | 2.77                     | 0.48              |
| 27:U:14:LEU:HD11 | 27:U:71:ALA:HB2   | 1.95                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:400:G:N7     | 30:X:57:ARG:NH1   | 2.57                     | 0.48              |
| 5:5:15:C:O2'     | 5:5:60:U:O3'      | 2.32                     | 0.48              |
| 14:H:56:ARG:HG2  | 14:H:83:ALA:HB2   | 1.95                     | 0.48              |
| 1:1:144:A:H2'    | 1:1:145:C:C6      | 2.49                     | 0.48              |
| 2:2:381:C:H2'    | 2:2:382:A:O4'     | 2.13                     | 0.48              |
| 2:2:604:G:H2'    | 2:2:605:U:O4'     | 2.14                     | 0.48              |
| 2:2:860:A:H2'    | 2:2:861:G:O4'     | 2.14                     | 0.48              |
| 15:I:78:LEU:HD22 | 15:I:108:ILE:CG2  | 2.44                     | 0.48              |
| 18:L:77:ILE:CD1  | 18:L:108:ALA:HB1  | 2.44                     | 0.48              |
| 29:W:37:ILE:HG22 | 29:W:38:VAL:HG23  | 1.95                     | 0.48              |
| 25:S:20:VAL:HG11 | 25:S:44:ALA:HA    | 1.95                     | 0.48              |
| 1:1:1913:A:C5    | 2:2:1494:G:C8     | 3.02                     | 0.47              |
| 2:2:1017:U:O2'   | 2:2:1018:G:O4'    | 2.32                     | 0.47              |
| 1:1:1814:G:H4'   | 8:B:51:THR:HG21   | 1.96                     | 0.47              |
| 1:1:819:A:C4     | 1:1:1189:A:C2     | 3.02                     | 0.47              |
| 2:2:1276:G:C2'   | 2:2:1277:C:H5'    | 2.44                     | 0.47              |
| 6:6:22:ASP:CG    | 6:6:23:PRO:HD2    | 2.34                     | 0.47              |
| 2:2:439:U:O2     | 2:2:440:C:C5      | 2.65                     | 0.47              |
| 11:E:25:VAL:O    | 11:E:28:VAL:HG12  | 2.14                     | 0.47              |
| 2:2:961:U:H3     | 2:2:974:A:H61     | 1.60                     | 0.47              |
| 9:C:156:PHE:CD1  | 16:J:81:ILE:HD13  | 2.49                     | 0.47              |
| 30:X:7:VAL:HG21  | 30:X:59:ILE:HD11  | 1.96                     | 0.47              |
| 1:1:1412:U:C4    | 1:1:1413:A:N7     | 2.82                     | 0.47              |
| 1:1:2315:G:O2'   | 1:1:2316:G:C8     | 2.65                     | 0.47              |
| 12:F:24:ILE:HD13 | 12:F:72:LEU:HD21  | 1.95                     | 0.47              |
| 27:U:94:ARG:CB   | 27:U:103:ILE:HD12 | 2.44                     | 0.47              |
| 2:2:1109:C:C3'   | 2:2:1109:C:C5'    | 2.92                     | 0.47              |
| 2:2:146:G:H2'    | 2:2:147:G:H5'     | 1.95                     | 0.47              |
| 9:C:156:PHE:CE1  | 16:J:81:ILE:HD13  | 2.50                     | 0.47              |
| 14:H:28:ALA:HB1  | 14:H:81:LEU:HD13  | 1.97                     | 0.47              |
| 1:1:1169:A:H5''  | 1:1:1169:A:N3     | 2.29                     | 0.47              |
| 1:1:1594:U:H2'   | 1:1:1595:C:C6     | 2.50                     | 0.47              |
| 1:1:2065:C:H4'   | 1:1:2251:OMG:HM21 | 1.95                     | 0.47              |
| 1:1:2298:A:C4    | 1:1:2321:U:C5     | 3.03                     | 0.47              |
| 7:7:83:LEU:HD21  | 7:7:95:THR:CG2    | 2.42                     | 0.47              |
| 1:1:1075:C:H2'   | 1:1:1076:C:O4'    | 2.14                     | 0.47              |
| 1:1:233:A:C6     | 1:1:234:U:C5      | 3.03                     | 0.47              |
| 7:7:30:LYS:CD    | 7:7:66:VAL:HG11   | 2.45                     | 0.47              |
| 1:1:2602:A:C6    | 7:7:254:VAL:HG22  | 2.50                     | 0.47              |
| 2:2:1382:C:H2'   | 2:2:1383:C:H5'    | 1.97                     | 0.47              |
| 23:Q:58:ARG:HA   | 23:Q:61:TRP:CE3   | 2.49                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:F:50:LEU:HD13 | 12:F:72:LEU:HD23  | 1.96                     | 0.47              |
| 13:G:66:ASN:OD1  | 13:G:134:VAL:HG23 | 2.15                     | 0.47              |
| 1:1:1433:A:H2'   | 1:1:1434:A:O4'    | 2.15                     | 0.46              |
| 1:1:1827:U:OP2   | 8:B:221:ARG:NE    | 2.48                     | 0.46              |
| 1:1:2547:A:H2'   | 1:1:2548:U:C6     | 2.50                     | 0.46              |
| 2:2:927:G:C2'    | 2:2:928:G:H5'     | 2.44                     | 0.46              |
| 9:C:48:ILE:HG23  | 9:C:84:LEU:HD11   | 1.97                     | 0.46              |
| 26:T:43:ILE:O    | 26:T:47:VAL:HG23  | 2.15                     | 0.46              |
| 2:2:1189:U:OP1   | 25:S:98:LYS:NZ    | 162.37                   | 0.46              |
| 12:F:35:ARG:CD   | 12:F:71:LEU:HD13  | 2.45                     | 0.46              |
| 1:1:826:U:O2'    | 18:L:53:GLY:HA3   | 2.15                     | 0.46              |
| 23:Q:65:ILE:CD1  | 23:Q:92:ARG:HB2   | 2.44                     | 0.46              |
| 1:1:1720:U:H2'   | 1:1:1721:G:O4'    | 2.16                     | 0.46              |
| 1:1:234:U:N3     | 1:1:429:A:C6      | 2.83                     | 0.46              |
| 9:C:25:THR:HG21  | 9:C:193:VAL:HG22  | 1.96                     | 0.46              |
| 14:H:23:LEU:HA   | 14:H:118:ILE:HG12 | 1.96                     | 0.46              |
| 20:N:9:GLN:O     | 20:N:17:ARG:NH2   | 2.49                     | 0.46              |
| 21:O:18:LEU:HD23 | 21:O:25:ARG:HD2   | 1.96                     | 0.46              |
| 1:1:1021:A:H3'   | 1:1:1021:A:N3     | 2.30                     | 0.46              |
| 1:1:2014:A:H2'   | 1:1:2015:A:C8     | 2.50                     | 0.46              |
| 2:2:1277:C:O2'   | 2:2:1278:G:OP2    | 2.32                     | 0.46              |
| 11:E:57:LEU:HD13 | 11:E:65:PRO:HB3   | 1.98                     | 0.46              |
| 2:2:1317:C:O2    | 30:X:37:ARG:NH2   | 153.98                   | 0.46              |
| 8:B:162:VAL:CG1  | 8:B:174:LEU:HD12  | 2.43                     | 0.46              |
| 2:2:16:A:OP2     | 6:6:41:ARG:NH1    | 2.49                     | 0.46              |
| 1:1:1070:A:N7    | 1:1:1096:A:O2'    | 2.48                     | 0.46              |
| 1:1:1913:A:N6    | 2:2:1494:G:C8     | 2.83                     | 0.46              |
| 2:2:1390:U:H2'   | 2:2:1391:U:C6     | 2.51                     | 0.46              |
| 2:2:109:A:H2'    | 2:2:326:G:N2      | 2.30                     | 0.46              |
| 9:C:152:PRO:HG3  | 9:C:156:PHE:CE1   | 2.49                     | 0.46              |
| 13:G:6:LEU:HD11  | 13:G:37:VAL:CG2   | 2.46                     | 0.46              |
| 15:I:82:ALA:HB2  | 15:I:108:ILE:HD11 | 1.98                     | 0.46              |
| 1:1:1614:A:N1    | 25:S:93:ALA:HB2   | 2.31                     | 0.46              |
| 1:1:2328:A:H2'   | 1:1:2329:U:C6     | 2.50                     | 0.46              |
| 1:1:742:A:C2     | 1:1:755:U:N3      | 2.78                     | 0.46              |
| 11:E:61:SER:O    | 11:E:63:GLN:N     | 2.48                     | 0.46              |
| 13:G:58:LEU:O    | 13:G:61:VAL:HG22  | 2.16                     | 0.46              |
| 21:O:39:VAL:HG11 | 21:O:87:ILE:HG21  | 1.98                     | 0.46              |
| 26:T:2:ILE:HD13  | 26:T:42:GLU:HA    | 1.96                     | 0.46              |
| 1:1:2092:U:N3    | 1:1:2225:A:O2'    | 2.49                     | 0.46              |
| 1:1:2788:C:H2'   | 1:1:2789:C:C6     | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:7:83:LEU:HD13   | 7:7:99:ALA:HB2    | 1.97                     | 0.46              |
| 26:T:61:LEU:C     | 26:T:61:LEU:HD12  | 2.36                     | 0.46              |
| 2:2:1518:MA6:C9   | 2:2:1519:MA6:H93  | 2.46                     | 0.46              |
| 18:L:77:ILE:HD11  | 18:L:108:ALA:HB1  | 1.98                     | 0.46              |
| 1:1:560:C:O2      | 23:Q:48:ARG:NH1   | 2.46                     | 0.45              |
| 19:M:96:ILE:HG21  | 19:M:126:ILE:HD12 | 1.98                     | 0.45              |
| 1:1:973:A:O4'     | 1:1:1188:U:C6     | 2.70                     | 0.45              |
| 1:1:2025:C:H2'    | 1:1:2026:U:C6     | 2.52                     | 0.45              |
| 1:1:2812:G:H2'    | 1:1:2813:A:O4'    | 2.16                     | 0.45              |
| 2:2:337:G:H2'     | 2:2:338:A:C8      | 2.51                     | 0.45              |
| 1:1:1588:G:C6     | 1:1:1589:U:O4     | 2.69                     | 0.45              |
| 11:E:40:VAL:O     | 11:E:40:VAL:HG22  | 2.16                     | 0.45              |
| 1:1:1405:U:H3     | 1:1:1597:A:H61    | 1.64                     | 0.45              |
| 1:1:565:C:H2'     | 1:1:566:U:O4'     | 2.17                     | 0.45              |
| 13:G:6:LEU:HD11   | 13:G:37:VAL:HG23  | 1.98                     | 0.45              |
| 14:H:79:PRO:O     | 14:H:80:THR:HG23  | 2.16                     | 0.45              |
| 21:O:51:ALA:HB3   | 21:O:78:VAL:HB    | 1.98                     | 0.45              |
| 10:D:131:THR:HG22 | 10:D:160:ALA:O    | 2.17                     | 0.45              |
| 10:D:145:ASP:HA   | 10:D:166:LYS:HB3  | 1.98                     | 0.45              |
| 1:1:1068:G:N2     | 1:1:1095:A:O3'    | 2.49                     | 0.45              |
| 1:1:2070:A:H2'    | 1:1:2071:A:O4'    | 2.16                     | 0.45              |
| 1:1:2273:A:H2'    | 1:1:2274:A:C8     | 2.51                     | 0.45              |
| 2:2:6:G:O2'       | 2:2:7:A:H8        | 2.00                     | 0.45              |
| 1:1:2694:G:H2'    | 1:1:2695:U:O4'    | 2.16                     | 0.45              |
| 2:2:1402:4OC:O2   | 2:2:1500:A:N1     | 2.50                     | 0.45              |
| 8:B:68:LYS:HA     | 8:B:151:GLY:HA2   | 1.99                     | 0.45              |
| 8:B:43:ARG:NH2    | 8:B:49:ILE:HD11   | 2.32                     | 0.45              |
| 21:O:35:ILE:HG21  | 21:O:71:ALA:HA    | 1.99                     | 0.45              |
| 1:1:526:A:O2'     | 1:1:2043:C:O2     | 2.32                     | 0.45              |
| 1:1:783:A:H8      | 1:1:1778:U:HO2'   | 1.62                     | 0.45              |
| 1:1:1877:A:H2'    | 1:1:1878:G:O4'    | 2.17                     | 0.45              |
| 14:H:35:VAL:O     | 14:H:39:THR:HG23  | 2.17                     | 0.45              |
| 2:2:215:C:H2'     | 2:2:216:U:O4'     | 2.16                     | 0.44              |
| 6:6:19:LEU:O      | 6:6:22:ASP:CB     | 2.65                     | 0.44              |
| 8:B:240:PHE:CD2   | 8:B:240:PHE:O     | 2.70                     | 0.44              |
| 12:F:17:VAL:CG1   | 12:F:26:ILE:HD12  | 6.39                     | 0.44              |
| 16:J:17:VAL:HG23  | 16:J:137:PRO:HB2  | 1.99                     | 0.44              |
| 1:1:1108:U:H2'    | 1:1:1109:C:C6     | 2.52                     | 0.44              |
| 1:1:234:U:C4      | 1:1:429:A:N6      | 2.82                     | 0.44              |
| 2:2:37:U:O2       | 2:2:547:A:C2      | 2.68                     | 0.44              |
| 2:2:842:U:H3'     | 2:2:843:U:C5'     | 2.47                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:7:149:GLU:HG3   | 7:7:179:VAL:HG11  | 1.99                     | 0.44              |
| 2:2:1175:G:O2'    | 2:2:1176:A:P      | 2.75                     | 0.44              |
| 25:S:36:LEU:HD13  | 25:S:48:LYS:CA    | 2.44                     | 0.44              |
| 1:1:2101:A:N6     | 1:1:2188:U:O4     | 2.50                     | 0.44              |
| 2:2:495:A:C6      | 2:2:496:A:N6      | 2.85                     | 0.44              |
| 2:2:49:U:O2       | 2:2:362:G:H1'     | 2.18                     | 0.44              |
| 1:1:2315:G:H4'    | 11:E:127:ASN:HD21 | 1.82                     | 0.44              |
| 1:1:1469:A:H2'    | 1:1:1470:A:C8     | 2.53                     | 0.44              |
| 20:N:28:LEU:HD23  | 20:N:48:VAL:HG21  | 1.99                     | 0.44              |
| 1:1:1519:G:H2'    | 1:1:1520:U:O4'    | 2.18                     | 0.44              |
| 1:1:1989:G:H2'    | 1:1:1990:C:O4'    | 2.17                     | 0.44              |
| 27:U:94:ARG:HB3   | 27:U:103:ILE:HD12 | 1.98                     | 0.44              |
| 2:2:397:A:N3      | 2:2:397:A:H3'     | 2.32                     | 0.44              |
| 13:G:55:GLU:HA    | 13:G:58:LEU:HD12  | 2.00                     | 0.44              |
| 17:K:123:LEU:HD21 | 22:P:70:VAL:HG11  | 1.99                     | 0.44              |
| 1:1:1590:A:C2'    | 1:1:1591:A:O4'    | 2.65                     | 0.44              |
| 1:1:2698:U:H2'    | 1:1:2699:C:C6     | 2.53                     | 0.44              |
| 2:2:978:A:O2'     | 2:2:1322:C:H5     | 2.01                     | 0.44              |
| 1:1:813:U:H2'     | 1:1:814:C:C6      | 2.53                     | 0.43              |
| 11:E:170:LEU:HA   | 11:E:170:LEU:HD23 | 1.91                     | 0.43              |
| 22:P:22:PRO:HD3   | 22:P:50:ILE:HD12  | 1.99                     | 0.43              |
| 1:1:754:U:C2      | 1:1:755:U:C5      | 3.07                     | 0.43              |
| 8:B:205:LEU:HB3   | 8:B:210:ALA:HB3   | 2.00                     | 0.43              |
| 8:B:210:ALA:HA    | 8:B:213:TRP:CE3   | 2.53                     | 0.43              |
| 1:1:476:G:H4'     | 1:1:502:A:N1      | 2.34                     | 0.43              |
| 2:2:789:U:O2'     | 2:2:791:G:N7      | 2.46                     | 0.43              |
| 2:2:946:A:H2'     | 2:2:947:G:C8      | 2.53                     | 0.43              |
| 17:K:21:CYS:HA    | 17:K:41:ILE:HG22  | 2.00                     | 0.43              |
| 1:1:2469:A:H4'    | 19:M:55:ARG:HD2   | 1.99                     | 0.43              |
| 1:1:1808:A:O2'    | 30:X:3:ARG:NH1    | 2.51                     | 0.43              |
| 1:1:2252:G:H2'    | 1:1:2253:G:C8     | 2.52                     | 0.43              |
| 1:1:2646:C:O5'    | 1:1:2646:C:H6     | 2.01                     | 0.43              |
| 1:1:2228:G:H2'    | 1:1:2229:U:C6     | 2.53                     | 0.43              |
| 1:1:2902:C:H2'    | 1:1:2903:U:H5'    | 2.00                     | 0.43              |
| 2:2:1176:A:H2'    | 2:2:1177:G:O4'    | 2.19                     | 0.43              |
| 2:2:384:G:H2'     | 2:2:385:C:C6      | 2.53                     | 0.43              |
| 3:3:89:U:O2       | 3:3:89:U:O4'      | 2.36                     | 0.43              |
| 17:K:76:VAL:HG12  | 22:P:73:VAL:HB    | 2.00                     | 0.43              |
| 2:2:421:U:O4'     | 2:2:421:U:O2      | 2.36                     | 0.43              |
| 1:1:1172:C:H2'    | 1:1:1173:U:O4'    | 2.18                     | 0.43              |
| 2:2:567:G:H2'     | 2:2:568:G:O4'     | 2.19                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 16:J:30:THR:CG2   | 16:J:31:GLU:N    | 2.82                     | 0.43              |
| 1:1:1406:U:O2'    | 1:1:1407:G:C5'   | 2.67                     | 0.43              |
| 31:Y:46:VAL:O     | 31:Y:50:VAL:HG23 | 2.19                     | 0.43              |
| 1:1:1400:U:H2'    | 1:1:1401:G:O4'   | 2.18                     | 0.43              |
| 1:1:2190:G:H2'    | 1:1:2191:A:O4'   | 2.19                     | 0.43              |
| 1:1:851:C:H2'     | 1:1:852:U:C6     | 2.54                     | 0.43              |
| 2:2:1236:A:H2'    | 2:2:1237:C:C6    | 2.54                     | 0.43              |
| 7:7:155:TRP:HH2   | 7:7:191:TRP:HB3  | 1.84                     | 0.43              |
| 1:1:2287:A:N3     | 1:1:2287:A:H2'   | 2.34                     | 0.43              |
| 2:2:1305:G:O2'    | 2:2:1306:A:H8    | 2.01                     | 0.43              |
| 16:J:32:LEU:CD2   | 16:J:54:ILE:HG21 | 2.49                     | 0.43              |
| 25:S:20:VAL:O     | 25:S:23:LEU:HB2  | 2.19                     | 0.43              |
| 1:1:1251:C:OP2    | 23:Q:6:ARG:NH2   | 2.51                     | 0.42              |
| 2:2:512:U:H2'     | 2:2:513:C:C6     | 2.54                     | 0.42              |
| 25:S:24:ILE:HD13  | 25:S:36:LEU:HD11 | 2.01                     | 0.42              |
| 2:2:1251:A:H2'    | 2:2:1252:A:O4'   | 2.18                     | 0.42              |
| 2:2:1277:C:C2'    | 2:2:1278:G:OP2   | 2.66                     | 0.42              |
| 2:2:1417:G:C6     | 2:2:1482:G:C6    | 3.08                     | 0.42              |
| 2:2:17:U:H2'      | 2:2:18:C:C6      | 2.54                     | 0.42              |
| 22:P:14:LYS:NZ    | 22:P:76:THR:O    | 2.52                     | 0.42              |
| 1:1:1590:A:H2'    | 1:1:1591:A:O4'   | 2.18                     | 0.42              |
| 1:1:1590:A:C4     | 1:1:1591:A:N7    | 2.87                     | 0.42              |
| 1:1:2133:G:O2'    | 1:1:2157:G:N2    | 2.52                     | 0.42              |
| 1:1:2788:C:O2'    | 1:1:2809:A:N3    | 2.49                     | 0.42              |
| 1:1:627:A:OP1     | 18:L:78:ARG:NH2  | 2.52                     | 0.42              |
| 2:2:915:A:N6      | 2:2:916:U:C4     | 2.87                     | 0.42              |
| 7:7:265:HIS:HB2   | 7:7:291:MET:CE   | 2.49                     | 0.42              |
| 24:R:5:PHE:HB3    | 24:R:59:ILE:HD12 | 2.01                     | 0.42              |
| 1:1:1009:A:N3     | 1:1:1153:C:O2'   | 2.47                     | 0.42              |
| 1:1:1915:3TD:H10B | 1:1:1916:A:N6    | 2.33                     | 0.42              |
| 1:1:523:C:H4'     | 1:1:540:C:O2     | 2.19                     | 0.42              |
| 1:1:57:C:H2'      | 1:1:58:G:O4'     | 2.18                     | 0.42              |
| 1:1:879:G:H2'     | 1:1:880:G:O4'    | 2.19                     | 0.42              |
| 2:2:1067:A:N1     | 2:2:1108:G:O2'   | 2.50                     | 0.42              |
| 2:2:1407:5MC:C2'  | 2:2:1408:A:H5'   | 2.50                     | 0.42              |
| 2:2:61:G:H2'      | 2:2:62:U:O4'     | 2.20                     | 0.42              |
| 2:2:146:G:H2'     | 2:2:147:G:C5'    | 2.49                     | 0.42              |
| 2:2:516:PSU:O2'   | 2:2:519:C:N3     | 2.52                     | 0.42              |
| 2:2:51:A:N7       | 2:2:114:U:O2'    | 2.49                     | 0.42              |
| 1:1:1796:U:H2'    | 1:1:1797:G:C8    | 2.54                     | 0.42              |
| 1:1:2032:G:H21    | 9:C:151:THR:HG23 | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:1098:C:H2'    | 2:2:1099:G:O4'    | 2.19                     | 0.42              |
| 7:7:240:ARG:HB2   | 7:7:266:ILE:HD11  | 2.01                     | 0.42              |
| 14:H:108:VAL:HG12 | 14:H:108:VAL:O    | 2.19                     | 0.42              |
| 1:1:1589:U:C2     | 1:1:1590:A:C8     | 3.07                     | 0.42              |
| 2:2:1486:G:H2'    | 2:2:1487:G:O4'    | 2.20                     | 0.42              |
| 7:7:249:ALA:HB1   | 7:7:254:VAL:HG11  | 2.02                     | 0.42              |
| 30:X:31:PRO:HG2   | 30:X:33:LEU:HD13  | 2.01                     | 0.42              |
| 1:1:2092:U:C2     | 1:1:2225:A:O2'    | 2.66                     | 0.42              |
| 1:1:745:1MG:HN21  | 1:1:745:1MG:HM11  | 1.67                     | 0.42              |
| 9:C:2:ILE:CD1     | 9:C:96:ILE:HD13   | 2.50                     | 0.42              |
| 1:1:1417:C:N3     | 1:1:1581:G:O6     | 2.53                     | 0.42              |
| 1:1:1824:G:O2'    | 8:B:252:THR:CG2   | 2.65                     | 0.42              |
| 1:1:1914:C:O2'    | 6:6:13:ASP:HB3    | 2.20                     | 0.42              |
| 1:1:323:C:C4      | 1:1:333:G:C8      | 3.07                     | 0.42              |
| 2:2:299:G:H2'     | 2:2:300:A:C8      | 2.54                     | 0.42              |
| 20:N:38:LEU:HB3   | 20:N:39:PRO:HD3   | 2.02                     | 0.42              |
| 22:P:106:LYS:HA   | 22:P:109:ARG:HD3  | 2.01                     | 0.42              |
| 1:1:44:A:H2'      | 1:1:45:G:O4'      | 2.20                     | 0.41              |
| 2:2:900:A:H2'     | 2:2:901:A:C8      | 2.55                     | 0.41              |
| 7:7:249:ALA:HB3   | 7:7:254:VAL:HG11  | 2.02                     | 0.41              |
| 15:I:102:ARG:HA   | 15:I:105:LEU:HD12 | 2.02                     | 0.41              |
| 30:X:4:VAL:HG22   | 30:X:11:ARG:HG2   | 2.01                     | 0.41              |
| 1:1:1009:A:O4'    | 23:Q:59:GLN:HG2   | 2.20                     | 0.41              |
| 1:1:2537:U:H2'    | 1:1:2538:C:C6     | 2.55                     | 0.41              |
| 1:1:833:A:H2'     | 1:1:834:G:C8      | 2.54                     | 0.41              |
| 7:7:268:THR:HG21  | 7:7:270:ILE:HD11  | 2.02                     | 0.41              |
| 1:1:1386:C:H2'    | 1:1:1387:A:C8     | 2.55                     | 0.41              |
| 1:1:1678:A:H2'    | 1:1:1679:A:O4'    | 2.20                     | 0.41              |
| 1:1:1739:A:H2'    | 1:1:1740:G:O4'    | 2.20                     | 0.41              |
| 2:2:922:G:N3      | 2:2:1398:A:H2     | 2.18                     | 0.41              |
| 2:2:767:A:H2'     | 2:2:768:A:O4'     | 2.20                     | 0.41              |
| 2:2:945:G:C2      | 2:2:946:A:C8      | 3.09                     | 0.41              |
| 16:J:76:HIS:CE1   | 16:J:85:LYS:HB2   | 2.55                     | 0.41              |
| 1:1:1125:G:C6     | 1:1:1126:A:N6     | 2.89                     | 0.41              |
| 1:1:1590:A:H2     | 1:1:1591:A:C2     | 2.38                     | 0.41              |
| 2:2:218:U:H2'     | 2:2:219:U:O4'     | 2.19                     | 0.41              |
| 9:C:77:ARG:NH2    | 9:C:200:ASP:OD1   | 2.53                     | 0.41              |
| 1:1:1595:C:C2'    | 1:1:1596:A:H5'    | 2.50                     | 0.41              |
| 9:C:32:ASN:HD22   | 9:C:32:ASN:N      | 2.19                     | 0.41              |
| 21:O:82:ALA:CB    | 21:O:115:LEU:HD21 | 2.49                     | 0.41              |
| 1:1:1433:A:H2'    | 1:1:1434:A:C1'    | 2.51                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:657:U:H2'    | 1:1:658:U:C6      | 2.55                     | 0.41              |
| 1:1:784:G:H5'    | 1:1:785:G:OP1     | 2.20                     | 0.41              |
| 1:1:910:A:N1     | 1:1:2277:G:H1'    | 2.35                     | 0.41              |
| 1:1:2315:G:H4'   | 11:E:127:ASN:ND2  | 2.36                     | 0.41              |
| 11:E:16:LEU:HD13 | 11:E:28:VAL:HG22  | 2.03                     | 0.41              |
| 20:N:21:PHE:CZ   | 20:N:43:GLU:HB3   | 2.56                     | 0.41              |
| 26:T:34:VAL:HG21 | 26:T:43:ILE:HD11  | 2.02                     | 0.41              |
| 27:U:5:ILE:N     | 27:U:5:ILE:HD12   | 2.35                     | 0.41              |
| 1:1:1405:U:H3    | 1:1:1597:A:N6     | 2.19                     | 0.41              |
| 1:1:1612:C:H2'   | 1:1:1613:G:O5'    | 2.21                     | 0.41              |
| 1:1:1783:A:N1    | 1:1:2587:A:H2'    | 2.35                     | 0.41              |
| 1:1:2557:G:H2'   | 1:1:2558:C:C6     | 2.55                     | 0.41              |
| 2:2:657:U:O2     | 26:T:22:THR:HG23  | 119.83                   | 0.41              |
| 5:5:19:G:H3'     | 5:5:20:H2U:H5''   | 2.03                     | 0.41              |
| 2:2:16:A:OP1     | 6:6:41:ARG:HG3    | 2.20                     | 0.41              |
| 25:S:4:ILE:HG12  | 25:S:106:VAL:HG22 | 2.02                     | 0.41              |
| 1:1:2074:U:H2'   | 1:1:2075:U:C6     | 2.56                     | 0.41              |
| 1:1:429:A:C2     | 1:1:430:A:C2      | 3.09                     | 0.41              |
| 1:1:861:A:C2     | 1:1:917:A:C4      | 3.09                     | 0.41              |
| 2:2:401:C:O2'    | 2:2:621:A:N3      | 2.48                     | 0.41              |
| 2:2:966:2MG:HM22 | 5:5:34:C:C5'      | 2.50                     | 0.41              |
| 27:U:85:PHE:CE1  | 27:U:94:ARG:HG2   | 2.56                     | 0.41              |
| 1:1:1327:A:H2'   | 1:1:1328:A:O4'    | 2.21                     | 0.41              |
| 2:2:1435:G:H2'   | 2:2:1436:U:C6     | 2.55                     | 0.41              |
| 18:L:95:LEU:HD11 | 18:L:125:LEU:HD21 | 2.03                     | 0.41              |
| 1:1:2607:G:H2'   | 1:1:2608:G:O4'    | 2.20                     | 0.41              |
| 2:2:956:U:H2'    | 2:2:957:U:O4'     | 2.20                     | 0.41              |
| 9:C:142:VAL:HB   | 9:C:143:PRO:HD2   | 2.01                     | 0.41              |
| 11:E:79:ILE:HG21 | 11:E:85:ILE:HD13  | 2.03                     | 0.41              |
| 20:N:28:LEU:O    | 20:N:32:GLU:N     | 2.53                     | 0.41              |
| 2:2:1389:C:C2'   | 2:2:1390:U:H5'    | 2.51                     | 0.41              |
| 19:M:77:PRO:HG2  | 19:M:80:VAL:HG21  | 2.03                     | 0.41              |
| 1:1:12:U:O2      | 1:1:12:U:H2'      | 2.21                     | 0.40              |
| 1:1:142:A:O2'    | 1:1:143:C:O4'     | 2.39                     | 0.40              |
| 2:2:1477:U:H2'   | 2:2:1478:U:C6     | 2.56                     | 0.40              |
| 7:7:326:TYR:CD2  | 7:7:333:ILE:HD12  | 2.57                     | 0.40              |
| 12:F:17:VAL:HG11 | 12:F:50:LEU:HD21  | 2.03                     | 0.40              |
| 15:I:37:PHE:CE1  | 15:I:58:ILE:HG23  | 2.57                     | 0.40              |
| 26:T:47:VAL:HG11 | 26:T:55:VAL:CG2   | 2.50                     | 0.40              |
| 26:T:30:ILE:HG21 | 26:T:93:LEU:HD13  | 2.03                     | 0.40              |
| 1:1:1853:A:N1    | 1:1:2087:G:H1'    | 2.36                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:257:C:H2'     | 1:1:258:G:O4'     | 2.21                     | 0.40              |
| 2:2:429:U:C2      | 2:2:431:A:C6      | 3.04                     | 0.40              |
| 2:2:949:A:H2'     | 2:2:950:U:O4'     | 2.21                     | 0.40              |
| 8:B:267:ILE:HG21  | 8:B:270:ARG:HD2   | 2.03                     | 0.40              |
| 8:B:37:ASN:HB2    | 8:B:62:TYR:HB2    | 2.04                     | 0.40              |
| 1:1:133:U:H2'     | 1:1:134:G:O4'     | 2.22                     | 0.40              |
| 1:1:1794:A:H2'    | 1:1:1795:C:C6     | 2.56                     | 0.40              |
| 1:1:2314:A:H1'    | 11:E:155:THR:HG21 | 2.04                     | 0.40              |
| 1:1:2327:A:H2'    | 1:1:2328:A:C8     | 2.56                     | 0.40              |
| 1:1:615:U:O4      | 10:D:39:ALA:HB2   | 2.22                     | 0.40              |
| 2:2:975:A:H8      | 2:2:1357:A:HO2'   | 1.67                     | 0.40              |
| 2:2:690:G:H2'     | 2:2:691:G:O4'     | 2.21                     | 0.40              |
| 8:B:172:VAL:HG23  | 8:B:174:LEU:CD2   | 2.51                     | 0.40              |
| 1:1:1083:U:O5'    | 14:H:41:LEU:HD22  | 2.21                     | 0.40              |
| 25:S:59:GLU:CD    | 25:S:66:ILE:HD11  | 2.41                     | 0.40              |
| 1:1:1596:A:O2'    | 1:1:1597:A:O5'    | 2.40                     | 0.40              |
| 1:1:247:G:N7      | 1:1:249:C:C2      | 2.89                     | 0.40              |
| 1:1:754:U:C2      | 1:1:755:U:C4      | 3.09                     | 0.40              |
| 2:2:108:G:N3      | 2:2:108:G:H5''    | 2.37                     | 0.40              |
| 2:2:1476:A:H2'    | 2:2:1477:U:O4'    | 2.22                     | 0.40              |
| 12:F:121:ILE:HD11 | 12:F:140:VAL:CG1  | 2.50                     | 0.40              |
| 18:L:74:THR:HG22  | 18:L:107:PHE:HB2  | 2.02                     | 0.40              |
| 23:Q:66:ASN:OD1   | 23:Q:70:ARG:NE    | 2.55                     | 0.40              |
| 2:2:1317:C:OP2    | 25:S:28:LYS:CE    | 197.91                   | 0.40              |
| 1:1:1406:U:O2'    | 1:1:1407:G:O4'    | 2.35                     | 0.40              |
| 1:1:742:A:N1      | 1:1:755:U:O4      | 2.54                     | 0.40              |
| 2:2:1428:A:H2'    | 2:2:1429:A:O4'    | 2.22                     | 0.40              |
| 2:2:975:A:N1      | 2:2:1366:C:O2'    | 2.42                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 6   | 6     | 44/61 (72%)   | 39 (89%)  | 5 (11%)  | 0        | 100         | 100 |
| 7   | 7     | 359/365 (98%) | 344 (96%) | 14 (4%)  | 1 (0%)   | 46          | 82  |
| 8   | B     | 269/273 (98%) | 255 (95%) | 13 (5%)  | 1 (0%)   | 39          | 79  |
| 9   | C     | 207/209 (99%) | 198 (96%) | 8 (4%)   | 1 (0%)   | 34          | 75  |
| 10  | D     | 199/201 (99%) | 190 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 11  | E     | 175/179 (98%) | 166 (95%) | 8 (5%)   | 1 (1%)   | 30          | 71  |
| 12  | F     | 173/177 (98%) | 161 (93%) | 12 (7%)  | 0        | 100         | 100 |
| 13  | G     | 147/149 (99%) | 133 (90%) | 14 (10%) | 0        | 100         | 100 |
| 14  | H     | 128/165 (78%) | 104 (81%) | 20 (16%) | 4 (3%)   | 5           | 26  |
| 15  | I     | 133/142 (94%) | 114 (86%) | 17 (13%) | 2 (2%)   | 13          | 48  |
| 16  | J     | 140/142 (99%) | 136 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 17  | K     | 121/123 (98%) | 116 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 18  | L     | 142/144 (99%) | 133 (94%) | 7 (5%)   | 2 (1%)   | 14          | 50  |
| 19  | M     | 134/136 (98%) | 130 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 20  | N     | 117/127 (92%) | 106 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 21  | O     | 114/117 (97%) | 109 (96%) | 4 (4%)   | 1 (1%)   | 21          | 63  |
| 22  | P     | 112/115 (97%) | 104 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 23  | Q     | 115/118 (98%) | 112 (97%) | 2 (2%)   | 1 (1%)   | 21          | 63  |
| 24  | R     | 101/103 (98%) | 98 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 25  | S     | 108/110 (98%) | 104 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 26  | T     | 92/100 (92%)  | 90 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 27  | U     | 101/104 (97%) | 97 (96%)  | 3 (3%)   | 1 (1%)   | 19          | 60  |
| 28  | V     | 92/94 (98%)   | 91 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 29  | W     | 74/85 (87%)   | 71 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 30  | X     | 75/78 (96%)   | 71 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 31  | Y     | 60/63 (95%)   | 59 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 32  | Z     | 56/59 (95%)   | 51 (91%)  | 5 (9%)   | 0        | 100         | 100 |
| 33  | a     | 64/70 (91%)   | 62 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 34  | b     | 54/57 (95%)   | 50 (93%)  | 4 (7%)   | 0        | 100         | 100 |
| 35  | c     | 50/55 (91%)   | 50 (100%) | 0        | 0        | 100         | 100 |
| 36  | d     | 44/46 (96%)   | 42 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 37  | e     | 62/65 (95%)   | 57 (92%)  | 5 (8%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 38  | f     | 36/38 (95%)     | 35 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 39  | g     | 223/241 (92%)   | 213 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 40  | h     | 206/233 (88%)   | 197 (96%)  | 6 (3%)   | 3 (2%)   | 13          | 48  |
| 41  | i     | 203/206 (98%)   | 194 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 42  | j     | 154/167 (92%)   | 145 (94%)  | 8 (5%)   | 1 (1%)   | 30          | 71  |
| 43  | k     | 102/135 (76%)   | 98 (96%)   | 3 (3%)   | 1 (1%)   | 19          | 60  |
| 44  | l     | 150/179 (84%)   | 143 (95%)  | 6 (4%)   | 1 (1%)   | 26          | 68  |
| 45  | m     | 127/130 (98%)   | 120 (94%)  | 6 (5%)   | 1 (1%)   | 24          | 65  |
| 46  | n     | 125/130 (96%)   | 116 (93%)  | 7 (6%)   | 2 (2%)   | 12          | 46  |
| 47  | o     | 97/103 (94%)    | 90 (93%)   | 6 (6%)   | 1 (1%)   | 19          | 60  |
| 48  | p     | 115/129 (89%)   | 104 (90%)  | 11 (10%) | 0        | 100         | 100 |
| 49  | q     | 120/124 (97%)   | 115 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 50  | r     | 114/118 (97%)   | 109 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 51  | s     | 98/101 (97%)    | 96 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 52  | t     | 86/89 (97%)     | 82 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 53  | u     | 80/82 (98%)     | 77 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 54  | v     | 78/84 (93%)     | 74 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 55  | w     | 64/75 (85%)     | 63 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 56  | x     | 81/92 (88%)     | 78 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 57  | y     | 84/87 (97%)     | 84 (100%)  | 0        | 0        | 100         | 100 |
| 58  | z     | 68/71 (96%)     | 67 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| All | All   | 6273/6646 (94%) | 5943 (95%) | 305 (5%) | 25 (0%)  | 43          | 79  |

All (25) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | L     | 36  | LYS  |
| 27  | U     | 7   | ARG  |
| 46  | n     | 56  | ASP  |
| 47  | o     | 57  | VAL  |
| 8   | B     | 240 | PHE  |
| 9   | C     | 149 | ASN  |
| 14  | H     | 117 | LEU  |
| 23  | Q     | 3   | ARG  |
| 44  | l     | 130 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | I     | 64  | ARG  |
| 18  | L     | 99  | ASN  |
| 40  | h     | 14  | ILE  |
| 11  | E     | 62  | GLY  |
| 40  | h     | 60  | PRO  |
| 40  | h     | 80  | LYS  |
| 14  | H     | 51  | TYR  |
| 14  | H     | 113 | PHE  |
| 21  | O     | 99  | TYR  |
| 43  | k     | 96  | VAL  |
| 45  | m     | 75  | ILE  |
| 14  | H     | 108 | VAL  |
| 7   | 7     | 351 | GLY  |
| 15  | I     | 12  | VAL  |
| 42  | j     | 27  | GLY  |
| 46  | n     | 50  | GLN  |

### 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 |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 6   | 6     | 39/51 (76%)    | 37 (95%)  | 2 (5%)   | 29          | 67 |
| 7   | 7     | 306/310 (99%)  | 275 (90%) | 31 (10%) | 9           | 33 |
| 8   | B     | 216/218 (99%)  | 204 (94%) | 12 (6%)  | 26          | 64 |
| 9   | C     | 164/164 (100%) | 159 (97%) | 5 (3%)   | 48          | 82 |
| 10  | D     | 165/165 (100%) | 150 (91%) | 15 (9%)  | 12          | 39 |
| 11  | E     | 148/150 (99%)  | 136 (92%) | 12 (8%)  | 15          | 45 |
| 12  | F     | 136/138 (99%)  | 128 (94%) | 8 (6%)   | 24          | 61 |
| 13  | G     | 114/114 (100%) | 103 (90%) | 11 (10%) | 10          | 36 |
| 14  | H     | 99/123 (80%)   | 86 (87%)  | 13 (13%) | 5           | 20 |
| 15  | I     | 104/110 (94%)  | 91 (88%)  | 13 (12%) | 6           | 22 |
| 16  | J     | 116/116 (100%) | 108 (93%) | 8 (7%)   | 19          | 55 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 17  | K     | 104/104 (100%) | 97 (93%)  | 7 (7%)   | 20          | 56 |
| 18  | L     | 103/103 (100%) | 95 (92%)  | 8 (8%)   | 16          | 47 |
| 19  | M     | 109/109 (100%) | 101 (93%) | 8 (7%)   | 17          | 51 |
| 20  | N     | 99/103 (96%)   | 93 (94%)  | 6 (6%)   | 23          | 60 |
| 21  | O     | 86/87 (99%)    | 81 (94%)  | 5 (6%)   | 25          | 62 |
| 22  | P     | 99/100 (99%)   | 92 (93%)  | 7 (7%)   | 18          | 53 |
| 23  | Q     | 89/90 (99%)    | 81 (91%)  | 8 (9%)   | 12          | 40 |
| 24  | R     | 84/84 (100%)   | 79 (94%)  | 5 (6%)   | 24          | 61 |
| 25  | S     | 93/93 (100%)   | 85 (91%)  | 8 (9%)   | 13          | 42 |
| 26  | T     | 81/84 (96%)    | 79 (98%)  | 2 (2%)   | 55          | 85 |
| 27  | U     | 84/85 (99%)    | 79 (94%)  | 5 (6%)   | 24          | 61 |
| 28  | V     | 78/78 (100%)   | 73 (94%)  | 5 (6%)   | 22          | 58 |
| 29  | W     | 58/63 (92%)    | 56 (97%)  | 2 (3%)   | 44          | 80 |
| 30  | X     | 67/68 (98%)    | 64 (96%)  | 3 (4%)   | 34          | 72 |
| 31  | Y     | 54/55 (98%)    | 51 (94%)  | 3 (6%)   | 26          | 64 |
| 32  | Z     | 48/49 (98%)    | 45 (94%)  | 3 (6%)   | 22          | 58 |
| 33  | a     | 59/62 (95%)    | 54 (92%)  | 5 (8%)   | 13          | 43 |
| 34  | b     | 47/48 (98%)    | 44 (94%)  | 3 (6%)   | 22          | 58 |
| 35  | c     | 47/49 (96%)    | 45 (96%)  | 2 (4%)   | 35          | 74 |
| 36  | d     | 38/38 (100%)   | 35 (92%)  | 3 (8%)   | 15          | 46 |
| 37  | e     | 51/52 (98%)    | 48 (94%)  | 3 (6%)   | 24          | 61 |
| 38  | f     | 34/34 (100%)   | 31 (91%)  | 3 (9%)   | 12          | 41 |
| 39  | g     | 187/199 (94%)  | 182 (97%) | 5 (3%)   | 52          | 84 |
| 40  | h     | 171/190 (90%)  | 160 (94%) | 11 (6%)  | 22          | 58 |
| 41  | i     | 172/173 (99%)  | 163 (95%) | 9 (5%)   | 29          | 67 |
| 42  | j     | 119/126 (94%)  | 105 (88%) | 14 (12%) | 6           | 25 |
| 43  | k     | 91/116 (78%)   | 84 (92%)  | 7 (8%)   | 16          | 48 |
| 44  | l     | 125/147 (85%)  | 113 (90%) | 12 (10%) | 10          | 36 |
| 45  | m     | 104/105 (99%)  | 100 (96%) | 4 (4%)   | 40          | 77 |
| 46  | n     | 105/107 (98%)  | 98 (93%)  | 7 (7%)   | 20          | 56 |
| 47  | o     | 86/90 (96%)    | 77 (90%)  | 9 (10%)  | 8           | 30 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 48  | p     | 90/99 (91%)     | 83 (92%)   | 7 (8%)   | 16          | 47 |
| 49  | q     | 102/103 (99%)   | 93 (91%)   | 9 (9%)   | 12          | 41 |
| 50  | r     | 94/96 (98%)     | 84 (89%)   | 10 (11%) | 8           | 30 |
| 51  | s     | 83/84 (99%)     | 77 (93%)   | 6 (7%)   | 18          | 52 |
| 52  | t     | 76/77 (99%)     | 65 (86%)   | 11 (14%) | 4           | 17 |
| 53  | u     | 65/65 (100%)    | 59 (91%)   | 6 (9%)   | 11          | 38 |
| 54  | v     | 74/78 (95%)     | 70 (95%)   | 4 (5%)   | 27          | 65 |
| 55  | w     | 57/65 (88%)     | 55 (96%)   | 2 (4%)   | 43          | 79 |
| 56  | x     | 72/79 (91%)     | 68 (94%)   | 4 (6%)   | 26          | 64 |
| 57  | y     | 65/66 (98%)     | 58 (89%)   | 7 (11%)  | 8           | 29 |
| 58  | z     | 60/61 (98%)     | 58 (97%)   | 2 (3%)   | 45          | 80 |
| All | All   | 5217/5423 (96%) | 4837 (93%) | 380 (7%) | 22          | 51 |

All (380) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 6     | 1   | MET  |
| 6   | 6     | 31  | LYS  |
| 7   | 7     | 4   | ILE  |
| 7   | 7     | 27  | TYR  |
| 7   | 7     | 42  | GLU  |
| 7   | 7     | 60  | ARG  |
| 7   | 7     | 71  | ASP  |
| 7   | 7     | 83  | LEU  |
| 7   | 7     | 86  | LEU  |
| 7   | 7     | 95  | THR  |
| 7   | 7     | 106 | LEU  |
| 7   | 7     | 107 | GLU  |
| 7   | 7     | 124 | ASP  |
| 7   | 7     | 127 | ASP  |
| 7   | 7     | 140 | GLU  |
| 7   | 7     | 149 | GLU  |
| 7   | 7     | 159 | ARG  |
| 7   | 7     | 164 | GLU  |
| 7   | 7     | 186 | ASP  |
| 7   | 7     | 195 | GLU  |
| 7   | 7     | 234 | ILE  |
| 7   | 7     | 245 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | 7     | 256 | ARG  |
| 7   | 7     | 265 | HIS  |
| 7   | 7     | 299 | GLU  |
| 7   | 7     | 300 | MET  |
| 7   | 7     | 303 | LYS  |
| 7   | 7     | 311 | GLU  |
| 7   | 7     | 312 | ASP  |
| 7   | 7     | 317 | ILE  |
| 7   | 7     | 337 | ARG  |
| 7   | 7     | 362 | LYS  |
| 7   | 7     | 365 | LEU  |
| 8   | B     | 52  | ARG  |
| 8   | B     | 130 | LEU  |
| 8   | B     | 156 | ARG  |
| 8   | B     | 189 | ARG  |
| 8   | B     | 195 | VAL  |
| 8   | B     | 202 | LEU  |
| 8   | B     | 203 | ARG  |
| 8   | B     | 204 | VAL  |
| 8   | B     | 205 | LEU  |
| 8   | B     | 242 | LYS  |
| 8   | B     | 252 | THR  |
| 8   | B     | 258 | ARG  |
| 9   | C     | 13  | ARG  |
| 9   | C     | 32  | ASN  |
| 9   | C     | 43  | ASP  |
| 9   | C     | 77  | ARG  |
| 9   | C     | 118 | PHE  |
| 10  | D     | 7   | ASP  |
| 10  | D     | 21  | ARG  |
| 10  | D     | 22  | ASP  |
| 10  | D     | 40  | ARG  |
| 10  | D     | 57  | LYS  |
| 10  | D     | 69  | ARG  |
| 10  | D     | 73  | ILE  |
| 10  | D     | 77  | ILE  |
| 10  | D     | 88  | ARG  |
| 10  | D     | 108 | ILE  |
| 10  | D     | 109 | LEU  |
| 10  | D     | 111 | GLU  |
| 10  | D     | 122 | GLU  |
| 10  | D     | 149 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | D     | 184 | ASP  |
| 11  | E     | 6   | ASP  |
| 11  | E     | 17  | MET  |
| 11  | E     | 40  | VAL  |
| 11  | E     | 47  | LYS  |
| 11  | E     | 57  | LEU  |
| 11  | E     | 80  | ARG  |
| 11  | E     | 115 | ARG  |
| 11  | E     | 117 | LEU  |
| 11  | E     | 123 | ASP  |
| 11  | E     | 133 | ARG  |
| 11  | E     | 140 | GLU  |
| 11  | E     | 152 | LEU  |
| 12  | F     | 25  | THR  |
| 12  | F     | 32  | GLU  |
| 12  | F     | 95  | ARG  |
| 12  | F     | 110 | SER  |
| 12  | F     | 141 | ILE  |
| 12  | F     | 155 | GLU  |
| 12  | F     | 166 | ASP  |
| 12  | F     | 176 | LYS  |
| 13  | G     | 1   | MET  |
| 13  | G     | 11  | ASN  |
| 13  | G     | 12  | LEU  |
| 13  | G     | 17  | ASP  |
| 13  | G     | 41  | LYS  |
| 13  | G     | 51  | ARG  |
| 13  | G     | 66  | ASN  |
| 13  | G     | 72  | ILE  |
| 13  | G     | 101 | ASP  |
| 13  | G     | 114 | GLU  |
| 13  | G     | 129 | GLU  |
| 14  | H     | 3   | LEU  |
| 14  | H     | 34  | THR  |
| 14  | H     | 54  | VAL  |
| 14  | H     | 57  | ASN  |
| 14  | H     | 65  | GLU  |
| 14  | H     | 74  | ASP  |
| 14  | H     | 80  | THR  |
| 14  | H     | 86  | MET  |
| 14  | H     | 94  | ARG  |
| 14  | H     | 107 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | H     | 109 | LYS  |
| 14  | H     | 117 | LEU  |
| 14  | H     | 123 | ILE  |
| 15  | I     | 8   | VAL  |
| 15  | I     | 10  | LEU  |
| 15  | I     | 11  | GLN  |
| 15  | I     | 20  | SER  |
| 15  | I     | 38  | CYS  |
| 15  | I     | 41  | PHE  |
| 15  | I     | 42  | ASN  |
| 15  | I     | 46  | ASP  |
| 15  | I     | 67  | THR  |
| 15  | I     | 78  | LEU  |
| 15  | I     | 81  | LYS  |
| 15  | I     | 135 | MET  |
| 15  | I     | 137 | LEU  |
| 16  | J     | 1   | MET  |
| 16  | J     | 30  | THR  |
| 16  | J     | 35  | ARG  |
| 16  | J     | 57  | LEU  |
| 16  | J     | 108 | MET  |
| 16  | J     | 123 | LYS  |
| 16  | J     | 129 | GLU  |
| 16  | J     | 142 | ILE  |
| 17  | K     | 18  | ARG  |
| 17  | K     | 35  | VAL  |
| 17  | K     | 41  | ILE  |
| 17  | K     | 58  | LEU  |
| 17  | K     | 67  | LYS  |
| 17  | K     | 99  | ILE  |
| 17  | K     | 111 | LYS  |
| 18  | L     | 4   | ASN  |
| 18  | L     | 30  | THR  |
| 18  | L     | 40  | SER  |
| 18  | L     | 48  | ARG  |
| 18  | L     | 67  | THR  |
| 18  | L     | 78  | ARG  |
| 18  | L     | 84  | LYS  |
| 18  | L     | 115 | GLU  |
| 19  | M     | 16  | ARG  |
| 19  | M     | 18  | ARG  |
| 19  | M     | 78  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | M     | 80  | VAL  |
| 19  | M     | 100 | LYS  |
| 19  | M     | 106 | ASP  |
| 19  | M     | 110 | GLU  |
| 19  | M     | 115 | GLU  |
| 20  | N     | 2   | ARG  |
| 20  | N     | 20  | MET  |
| 20  | N     | 51  | LEU  |
| 20  | N     | 63  | ARG  |
| 20  | N     | 65  | LEU  |
| 20  | N     | 69  | ARG  |
| 21  | O     | 13  | ARG  |
| 21  | O     | 19  | GLN  |
| 21  | O     | 47  | VAL  |
| 21  | O     | 48  | LEU  |
| 21  | O     | 116 | GLN  |
| 22  | P     | 26  | VAL  |
| 22  | P     | 80  | VAL  |
| 22  | P     | 88  | ARG  |
| 22  | P     | 104 | THR  |
| 22  | P     | 111 | LYS  |
| 22  | P     | 113 | ARG  |
| 22  | P     | 114 | LEU  |
| 23  | Q     | 11  | ARG  |
| 23  | Q     | 18  | LEU  |
| 23  | Q     | 20  | GLN  |
| 23  | Q     | 51  | ARG  |
| 23  | Q     | 52  | GLN  |
| 23  | Q     | 59  | GLN  |
| 23  | Q     | 91  | ASP  |
| 23  | Q     | 117 | LEU  |
| 24  | R     | 10  | LYS  |
| 24  | R     | 39  | LEU  |
| 24  | R     | 48  | LYS  |
| 24  | R     | 79  | ARG  |
| 24  | R     | 86  | GLN  |
| 25  | S     | 19  | LEU  |
| 25  | S     | 41  | LYS  |
| 25  | S     | 67  | ASP  |
| 25  | S     | 69  | LEU  |
| 25  | S     | 83  | LYS  |
| 25  | S     | 97  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | S     | 109 | ASP  |
| 25  | S     | 110 | ARG  |
| 26  | T     | 1   | MET  |
| 26  | T     | 89  | GLU  |
| 27  | U     | 7   | ARG  |
| 27  | U     | 9   | ASP  |
| 27  | U     | 46  | GLN  |
| 27  | U     | 52  | LEU  |
| 27  | U     | 72  | ILE  |
| 28  | V     | 1   | MET  |
| 28  | V     | 34  | LYS  |
| 28  | V     | 40  | ILE  |
| 28  | V     | 41  | GLU  |
| 28  | V     | 45  | ASP  |
| 29  | W     | 11  | ARG  |
| 29  | W     | 70  | GLU  |
| 30  | X     | 44  | LYS  |
| 30  | X     | 48  | THR  |
| 30  | X     | 60  | ASP  |
| 31  | Y     | 7   | ARG  |
| 31  | Y     | 57  | LEU  |
| 31  | Y     | 58  | ASN  |
| 32  | Z     | 10  | THR  |
| 32  | Z     | 19  | LYS  |
| 32  | Z     | 45  | ARG  |
| 33  | a     | 37  | CYS  |
| 33  | a     | 40  | CYS  |
| 33  | a     | 43  | PHE  |
| 33  | a     | 47  | LYS  |
| 33  | a     | 59  | ARG  |
| 34  | b     | 12  | LYS  |
| 34  | b     | 40  | ARG  |
| 34  | b     | 55  | ILE  |
| 35  | c     | 5   | ILE  |
| 35  | c     | 32  | GLU  |
| 36  | d     | 22  | MET  |
| 36  | d     | 25  | LYS  |
| 36  | d     | 42  | LEU  |
| 37  | e     | 30  | ARG  |
| 37  | e     | 31  | HIS  |
| 37  | e     | 55  | LEU  |
| 38  | f     | 3   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | f     | 26  | ILE  |
| 38  | f     | 37  | GLN  |
| 39  | g     | 23  | TRP  |
| 39  | g     | 105 | LYS  |
| 39  | g     | 129 | LEU  |
| 39  | g     | 132 | LYS  |
| 39  | g     | 220 | THR  |
| 40  | h     | 14  | ILE  |
| 40  | h     | 35  | SER  |
| 40  | h     | 89  | LYS  |
| 40  | h     | 154 | SER  |
| 40  | h     | 164 | ARG  |
| 40  | h     | 165 | THR  |
| 40  | h     | 172 | ARG  |
| 40  | h     | 175 | LEU  |
| 40  | h     | 178 | LEU  |
| 40  | h     | 185 | ASN  |
| 40  | h     | 200 | VAL  |
| 41  | i     | 47  | ARG  |
| 41  | i     | 58  | LYS  |
| 41  | i     | 95  | GLU  |
| 41  | i     | 104 | ARG  |
| 41  | i     | 116 | GLN  |
| 41  | i     | 138 | SER  |
| 41  | i     | 143 | VAL  |
| 41  | i     | 197 | GLU  |
| 41  | i     | 206 | LYS  |
| 42  | j     | 15  | LEU  |
| 42  | j     | 18  | VAL  |
| 42  | j     | 46  | VAL  |
| 42  | j     | 60  | ILE  |
| 42  | j     | 65  | GLU  |
| 42  | j     | 93  | ARG  |
| 42  | j     | 114 | VAL  |
| 42  | j     | 115 | LEU  |
| 42  | j     | 120 | VAL  |
| 42  | j     | 123 | VAL  |
| 42  | j     | 138 | ARG  |
| 42  | j     | 141 | ILE  |
| 42  | j     | 142 | ASP  |
| 42  | j     | 146 | ASN  |
| 43  | k     | 7   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | k     | 16  | GLU  |
| 43  | k     | 24  | ARG  |
| 43  | k     | 38  | ARG  |
| 43  | k     | 54  | LEU  |
| 43  | k     | 79  | ARG  |
| 43  | k     | 86  | ARG  |
| 44  | l     | 7   | ILE  |
| 44  | l     | 17  | LYS  |
| 44  | l     | 21  | GLU  |
| 44  | l     | 23  | LEU  |
| 44  | l     | 27  | VAL  |
| 44  | l     | 50  | LEU  |
| 44  | l     | 79  | ARG  |
| 44  | l     | 80  | VAL  |
| 44  | l     | 109 | ARG  |
| 44  | l     | 123 | GLU  |
| 44  | l     | 130 | ASN  |
| 44  | l     | 146 | GLU  |
| 45  | m     | 3   | MET  |
| 45  | m     | 77  | ARG  |
| 45  | m     | 96  | MET  |
| 45  | m     | 121 | LEU  |
| 46  | n     | 12  | ARG  |
| 46  | n     | 41  | ARG  |
| 46  | n     | 57  | MET  |
| 46  | n     | 63  | LEU  |
| 46  | n     | 98  | LEU  |
| 46  | n     | 118 | LEU  |
| 46  | n     | 123 | ARG  |
| 47  | o     | 5   | ARG  |
| 47  | o     | 6   | ILE  |
| 47  | o     | 7   | ARG  |
| 47  | o     | 17  | LEU  |
| 47  | o     | 24  | GLU  |
| 47  | o     | 25  | ILE  |
| 47  | o     | 27  | GLU  |
| 47  | o     | 37  | ARG  |
| 47  | o     | 57  | VAL  |
| 48  | p     | 13  | ARG  |
| 48  | p     | 14  | LYS  |
| 48  | p     | 15  | GLN  |
| 48  | p     | 37  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | p     | 76  | GLU  |
| 48  | p     | 100 | LEU  |
| 48  | p     | 107 | ILE  |
| 49  | q     | 5   | ASN  |
| 49  | q     | 24  | LEU  |
| 49  | q     | 40  | THR  |
| 49  | q     | 43  | LYS  |
| 49  | q     | 44  | LYS  |
| 49  | q     | 47  | SER  |
| 49  | q     | 62  | GLU  |
| 49  | q     | 64  | THR  |
| 49  | q     | 102 | LEU  |
| 50  | r     | 11  | ASP  |
| 50  | r     | 16  | VAL  |
| 50  | r     | 25  | VAL  |
| 50  | r     | 29  | ARG  |
| 50  | r     | 59  | GLU  |
| 50  | r     | 89  | LEU  |
| 50  | r     | 92  | ARG  |
| 50  | r     | 93  | ARG  |
| 50  | r     | 96  | PRO  |
| 50  | r     | 104 | THR  |
| 51  | s     | 45  | VAL  |
| 51  | s     | 46  | LEU  |
| 51  | s     | 52  | PRO  |
| 51  | s     | 89  | MET  |
| 51  | s     | 92  | GLU  |
| 51  | s     | 100 | SER  |
| 52  | t     | 22  | THR  |
| 52  | t     | 39  | LEU  |
| 52  | t     | 40  | GLN  |
| 52  | t     | 61  | SER  |
| 52  | t     | 64  | ARG  |
| 52  | t     | 66  | LEU  |
| 52  | t     | 67  | LEU  |
| 52  | t     | 70  | LEU  |
| 52  | t     | 80  | GLN  |
| 52  | t     | 84  | ARG  |
| 52  | t     | 85  | LEU  |
| 53  | u     | 1   | MET  |
| 53  | u     | 6   | LEU  |
| 53  | u     | 18  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | u     | 19  | VAL  |
| 53  | u     | 50  | THR  |
| 53  | u     | 77  | GLU  |
| 54  | v     | 33  | ILE  |
| 54  | v     | 53  | CYS  |
| 54  | v     | 67  | LEU  |
| 54  | v     | 75  | LEU  |
| 55  | w     | 71  | THR  |
| 55  | w     | 74  | HIS  |
| 56  | x     | 21  | LYS  |
| 56  | x     | 33  | THR  |
| 56  | x     | 49  | ILE  |
| 56  | x     | 79  | THR  |
| 57  | y     | 6   | SER  |
| 57  | y     | 10  | ARG  |
| 57  | y     | 15  | GLU  |
| 57  | y     | 43  | ASP  |
| 57  | y     | 48  | GLN  |
| 57  | y     | 54  | MET  |
| 57  | y     | 64  | LYS  |
| 58  | z     | 4   | ILE  |
| 58  | z     | 67  | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1     | 2898/2904 (99%) | 556 (19%)         | 81 (2%)         |
| 2   | 2     | 1528/1534 (99%) | 295 (19%)         | 37 (2%)         |
| 3   | 3     | 119/120 (99%)   | 15 (12%)          | 0               |
| 4   | 4     | 4/18 (22%)      | 1 (25%)           | 0               |
| 5   | 5     | 73/78 (93%)     | 23 (31%)          | 9 (12%)         |
| All | All   | 4622/4654 (99%) | 890 (19%)         | 127 (2%)        |

All (890) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 10  | A    |
| 1   | 1     | 14  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 23  | G    |
| 1   | 1     | 34  | U    |
| 1   | 1     | 35  | G    |
| 1   | 1     | 45  | G    |
| 1   | 1     | 46  | G    |
| 1   | 1     | 58  | G    |
| 1   | 1     | 60  | G    |
| 1   | 1     | 62  | U    |
| 1   | 1     | 63  | A    |
| 1   | 1     | 71  | A    |
| 1   | 1     | 74  | A    |
| 1   | 1     | 75  | G    |
| 1   | 1     | 83  | A    |
| 1   | 1     | 84  | A    |
| 1   | 1     | 85  | G    |
| 1   | 1     | 99  | U    |
| 1   | 1     | 101 | A    |
| 1   | 1     | 102 | U    |
| 1   | 1     | 110 | G    |
| 1   | 1     | 118 | A    |
| 1   | 1     | 119 | A    |
| 1   | 1     | 120 | U    |
| 1   | 1     | 122 | G    |
| 1   | 1     | 131 | A    |
| 1   | 1     | 138 | U    |
| 1   | 1     | 139 | U    |
| 1   | 1     | 140 | C    |
| 1   | 1     | 141 | G    |
| 1   | 1     | 142 | A    |
| 1   | 1     | 144 | A    |
| 1   | 1     | 149 | A    |
| 1   | 1     | 163 | C    |
| 1   | 1     | 165 | A    |
| 1   | 1     | 181 | A    |
| 1   | 1     | 196 | A    |
| 1   | 1     | 200 | U    |
| 1   | 1     | 215 | G    |
| 1   | 1     | 216 | A    |
| 1   | 1     | 221 | A    |
| 1   | 1     | 222 | A    |
| 1   | 1     | 248 | G    |
| 1   | 1     | 249 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 264 | C    |
| 1   | 1     | 265 | A    |
| 1   | 1     | 266 | G    |
| 1   | 1     | 270 | A    |
| 1   | 1     | 271 | G    |
| 1   | 1     | 272 | A    |
| 1   | 1     | 275 | C    |
| 1   | 1     | 276 | U    |
| 1   | 1     | 278 | A    |
| 1   | 1     | 285 | G    |
| 1   | 1     | 310 | A    |
| 1   | 1     | 311 | A    |
| 1   | 1     | 327 | G    |
| 1   | 1     | 329 | G    |
| 1   | 1     | 330 | A    |
| 1   | 1     | 353 | C    |
| 1   | 1     | 361 | G    |
| 1   | 1     | 362 | A    |
| 1   | 1     | 371 | A    |
| 1   | 1     | 372 | G    |
| 1   | 1     | 386 | G    |
| 1   | 1     | 396 | G    |
| 1   | 1     | 405 | U    |
| 1   | 1     | 411 | G    |
| 1   | 1     | 412 | A    |
| 1   | 1     | 424 | G    |
| 1   | 1     | 435 | C    |
| 1   | 1     | 451 | U    |
| 1   | 1     | 456 | C    |
| 1   | 1     | 457 | A    |
| 1   | 1     | 477 | A    |
| 1   | 1     | 480 | A    |
| 1   | 1     | 481 | G    |
| 1   | 1     | 491 | G    |
| 1   | 1     | 501 | A    |
| 1   | 1     | 503 | A    |
| 1   | 1     | 504 | A    |
| 1   | 1     | 505 | A    |
| 1   | 1     | 508 | A    |
| 1   | 1     | 509 | C    |
| 1   | 1     | 531 | C    |
| 1   | 1     | 532 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 533 | G    |
| 1   | 1     | 543 | G    |
| 1   | 1     | 546 | U    |
| 1   | 1     | 547 | A    |
| 1   | 1     | 549 | G    |
| 1   | 1     | 551 | G    |
| 1   | 1     | 563 | A    |
| 1   | 1     | 569 | U    |
| 1   | 1     | 573 | U    |
| 1   | 1     | 574 | A    |
| 1   | 1     | 575 | A    |
| 1   | 1     | 586 | A    |
| 1   | 1     | 603 | A    |
| 1   | 1     | 609 | A    |
| 1   | 1     | 613 | A    |
| 1   | 1     | 614 | A    |
| 1   | 1     | 615 | U    |
| 1   | 1     | 616 | A    |
| 1   | 1     | 618 | G    |
| 1   | 1     | 627 | A    |
| 1   | 1     | 637 | A    |
| 1   | 1     | 645 | C    |
| 1   | 1     | 647 | G    |
| 1   | 1     | 651 | G    |
| 1   | 1     | 654 | A    |
| 1   | 1     | 655 | A    |
| 1   | 1     | 668 | A    |
| 1   | 1     | 686 | U    |
| 1   | 1     | 696 | G    |
| 1   | 1     | 710 | U    |
| 1   | 1     | 717 | C    |
| 1   | 1     | 724 | U    |
| 1   | 1     | 730 | A    |
| 1   | 1     | 738 | G    |
| 1   | 1     | 746 | PSU  |
| 1   | 1     | 747 | 5MU  |
| 1   | 1     | 757 | G    |
| 1   | 1     | 764 | A    |
| 1   | 1     | 765 | C    |
| 1   | 1     | 775 | G    |
| 1   | 1     | 776 | G    |
| 1   | 1     | 782 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 783 | A    |
| 1   | 1     | 784 | G    |
| 1   | 1     | 785 | G    |
| 1   | 1     | 788 | A    |
| 1   | 1     | 789 | A    |
| 1   | 1     | 805 | G    |
| 1   | 1     | 812 | C    |
| 1   | 1     | 819 | A    |
| 1   | 1     | 827 | U    |
| 1   | 1     | 828 | U    |
| 1   | 1     | 845 | A    |
| 1   | 1     | 846 | U    |
| 1   | 1     | 858 | G    |
| 1   | 1     | 859 | G    |
| 1   | 1     | 869 | G    |
| 1   | 1     | 878 | A    |
| 1   | 1     | 881 | G    |
| 1   | 1     | 884 | U    |
| 1   | 1     | 885 | C    |
| 1   | 1     | 887 | A    |
| 1   | 1     | 891 | G    |
| 1   | 1     | 892 | A    |
| 1   | 1     | 893 | C    |
| 1   | 1     | 895 | U    |
| 1   | 1     | 896 | A    |
| 1   | 1     | 897 | C    |
| 1   | 1     | 899 | A    |
| 1   | 1     | 910 | A    |
| 1   | 1     | 914 | G    |
| 1   | 1     | 915 | C    |
| 1   | 1     | 931 | U    |
| 1   | 1     | 933 | A    |
| 1   | 1     | 940 | G    |
| 1   | 1     | 941 | A    |
| 1   | 1     | 945 | A    |
| 1   | 1     | 946 | C    |
| 1   | 1     | 953 | G    |
| 1   | 1     | 961 | C    |
| 1   | 1     | 974 | G    |
| 1   | 1     | 983 | A    |
| 1   | 1     | 984 | A    |
| 1   | 1     | 985 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 995  | C    |
| 1   | 1     | 996  | A    |
| 1   | 1     | 999  | U    |
| 1   | 1     | 1005 | C    |
| 1   | 1     | 1012 | U    |
| 1   | 1     | 1013 | C    |
| 1   | 1     | 1023 | U    |
| 1   | 1     | 1026 | G    |
| 1   | 1     | 1033 | U    |
| 1   | 1     | 1040 | A    |
| 1   | 1     | 1043 | C    |
| 1   | 1     | 1045 | C    |
| 1   | 1     | 1046 | A    |
| 1   | 1     | 1047 | G    |
| 1   | 1     | 1050 | A    |
| 1   | 1     | 1055 | G    |
| 1   | 1     | 1060 | U    |
| 1   | 1     | 1061 | U    |
| 1   | 1     | 1063 | G    |
| 1   | 1     | 1064 | C    |
| 1   | 1     | 1065 | U    |
| 1   | 1     | 1066 | U    |
| 1   | 1     | 1067 | A    |
| 1   | 1     | 1068 | G    |
| 1   | 1     | 1069 | A    |
| 1   | 1     | 1070 | A    |
| 1   | 1     | 1073 | A    |
| 1   | 1     | 1074 | G    |
| 1   | 1     | 1083 | U    |
| 1   | 1     | 1084 | A    |
| 1   | 1     | 1087 | G    |
| 1   | 1     | 1088 | A    |
| 1   | 1     | 1090 | A    |
| 1   | 1     | 1107 | G    |
| 1   | 1     | 1111 | A    |
| 1   | 1     | 1112 | G    |
| 1   | 1     | 1119 | U    |
| 1   | 1     | 1122 | G    |
| 1   | 1     | 1128 | G    |
| 1   | 1     | 1129 | A    |
| 1   | 1     | 1130 | U    |
| 1   | 1     | 1132 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1134 | A    |
| 1   | 1     | 1135 | C    |
| 1   | 1     | 1142 | A    |
| 1   | 1     | 1169 | A    |
| 1   | 1     | 1170 | C    |
| 1   | 1     | 1171 | G    |
| 1   | 1     | 1173 | U    |
| 1   | 1     | 1174 | U    |
| 1   | 1     | 1175 | A    |
| 1   | 1     | 1176 | U    |
| 1   | 1     | 1177 | G    |
| 1   | 1     | 1178 | C    |
| 1   | 1     | 1179 | G    |
| 1   | 1     | 1180 | U    |
| 1   | 1     | 1186 | G    |
| 1   | 1     | 1236 | G    |
| 1   | 1     | 1238 | G    |
| 1   | 1     | 1248 | G    |
| 1   | 1     | 1253 | A    |
| 1   | 1     | 1256 | G    |
| 1   | 1     | 1265 | A    |
| 1   | 1     | 1266 | G    |
| 1   | 1     | 1271 | G    |
| 1   | 1     | 1272 | A    |
| 1   | 1     | 1273 | U    |
| 1   | 1     | 1300 | G    |
| 1   | 1     | 1301 | A    |
| 1   | 1     | 1302 | A    |
| 1   | 1     | 1321 | A    |
| 1   | 1     | 1345 | C    |
| 1   | 1     | 1352 | U    |
| 1   | 1     | 1365 | A    |
| 1   | 1     | 1368 | G    |
| 1   | 1     | 1378 | A    |
| 1   | 1     | 1379 | U    |
| 1   | 1     | 1380 | G    |
| 1   | 1     | 1383 | A    |
| 1   | 1     | 1395 | A    |
| 1   | 1     | 1405 | U    |
| 1   | 1     | 1406 | U    |
| 1   | 1     | 1407 | G    |
| 1   | 1     | 1408 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1409 | U    |
| 1   | 1     | 1414 | C    |
| 1   | 1     | 1416 | G    |
| 1   | 1     | 1417 | C    |
| 1   | 1     | 1420 | A    |
| 1   | 1     | 1428 | C    |
| 1   | 1     | 1434 | A    |
| 1   | 1     | 1452 | G    |
| 1   | 1     | 1453 | A    |
| 1   | 1     | 1455 | G    |
| 1   | 1     | 1458 | U    |
| 1   | 1     | 1460 | U    |
| 1   | 1     | 1478 | G    |
| 1   | 1     | 1482 | G    |
| 1   | 1     | 1483 | G    |
| 1   | 1     | 1490 | A    |
| 1   | 1     | 1493 | C    |
| 1   | 1     | 1497 | U    |
| 1   | 1     | 1503 | A    |
| 1   | 1     | 1508 | A    |
| 1   | 1     | 1509 | A    |
| 1   | 1     | 1510 | G    |
| 1   | 1     | 1515 | A    |
| 1   | 1     | 1529 | G    |
| 1   | 1     | 1534 | U    |
| 1   | 1     | 1535 | A    |
| 1   | 1     | 1536 | C    |
| 1   | 1     | 1537 | G    |
| 1   | 1     | 1554 | U    |
| 1   | 1     | 1558 | C    |
| 1   | 1     | 1559 | U    |
| 1   | 1     | 1566 | A    |
| 1   | 1     | 1569 | A    |
| 1   | 1     | 1578 | U    |
| 1   | 1     | 1580 | A    |
| 1   | 1     | 1581 | G    |
| 1   | 1     | 1583 | A    |
| 1   | 1     | 1584 | U    |
| 1   | 1     | 1589 | U    |
| 1   | 1     | 1590 | A    |
| 1   | 1     | 1592 | C    |
| 1   | 1     | 1593 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1594 | U    |
| 1   | 1     | 1595 | C    |
| 1   | 1     | 1596 | A    |
| 1   | 1     | 1597 | A    |
| 1   | 1     | 1608 | A    |
| 1   | 1     | 1609 | A    |
| 1   | 1     | 1610 | A    |
| 1   | 1     | 1613 | G    |
| 1   | 1     | 1619 | G    |
| 1   | 1     | 1630 | A    |
| 1   | 1     | 1647 | U    |
| 1   | 1     | 1648 | U    |
| 1   | 1     | 1649 | G    |
| 1   | 1     | 1651 | G    |
| 1   | 1     | 1674 | G    |
| 1   | 1     | 1677 | A    |
| 1   | 1     | 1703 | G    |
| 1   | 1     | 1713 | A    |
| 1   | 1     | 1714 | U    |
| 1   | 1     | 1715 | G    |
| 1   | 1     | 1718 | G    |
| 1   | 1     | 1729 | U    |
| 1   | 1     | 1730 | C    |
| 1   | 1     | 1732 | C    |
| 1   | 1     | 1738 | G    |
| 1   | 1     | 1742 | U    |
| 1   | 1     | 1750 | G    |
| 1   | 1     | 1755 | A    |
| 1   | 1     | 1758 | U    |
| 1   | 1     | 1761 | C    |
| 1   | 1     | 1764 | C    |
| 1   | 1     | 1773 | A    |
| 1   | 1     | 1791 | A    |
| 1   | 1     | 1800 | C    |
| 1   | 1     | 1801 | A    |
| 1   | 1     | 1808 | A    |
| 1   | 1     | 1811 | G    |
| 1   | 1     | 1816 | C    |
| 1   | 1     | 1829 | A    |
| 1   | 1     | 1833 | C    |
| 1   | 1     | 1848 | A    |
| 1   | 1     | 1858 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1859 | U    |
| 1   | 1     | 1862 | G    |
| 1   | 1     | 1864 | U    |
| 1   | 1     | 1869 | G    |
| 1   | 1     | 1870 | C    |
| 1   | 1     | 1872 | A    |
| 1   | 1     | 1873 | G    |
| 1   | 1     | 1905 | C    |
| 1   | 1     | 1906 | G    |
| 1   | 1     | 1907 | G    |
| 1   | 1     | 1912 | A    |
| 1   | 1     | 1913 | A    |
| 1   | 1     | 1914 | C    |
| 1   | 1     | 1917 | PSU  |
| 1   | 1     | 1918 | A    |
| 1   | 1     | 1919 | A    |
| 1   | 1     | 1929 | G    |
| 1   | 1     | 1930 | G    |
| 1   | 1     | 1931 | U    |
| 1   | 1     | 1936 | A    |
| 1   | 1     | 1938 | A    |
| 1   | 1     | 1939 | 5MU  |
| 1   | 1     | 1955 | U    |
| 1   | 1     | 1960 | A    |
| 1   | 1     | 1963 | U    |
| 1   | 1     | 1965 | C    |
| 1   | 1     | 1966 | A    |
| 1   | 1     | 1967 | C    |
| 1   | 1     | 1970 | A    |
| 1   | 1     | 1971 | U    |
| 1   | 1     | 1972 | G    |
| 1   | 1     | 1987 | A    |
| 1   | 1     | 1991 | U    |
| 1   | 1     | 1992 | G    |
| 1   | 1     | 1993 | U    |
| 1   | 1     | 1997 | C    |
| 1   | 1     | 2002 | G    |
| 1   | 1     | 2022 | U    |
| 1   | 1     | 2023 | C    |
| 1   | 1     | 2026 | U    |
| 1   | 1     | 2031 | A    |
| 1   | 1     | 2033 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2043 | C    |
| 1   | 1     | 2051 | A    |
| 1   | 1     | 2052 | A    |
| 1   | 1     | 2055 | C    |
| 1   | 1     | 2056 | G    |
| 1   | 1     | 2060 | A    |
| 1   | 1     | 2061 | G    |
| 1   | 1     | 2062 | A    |
| 1   | 1     | 2063 | C    |
| 1   | 1     | 2069 | G7M  |
| 1   | 1     | 2097 | A    |
| 1   | 1     | 2099 | U    |
| 1   | 1     | 2100 | G    |
| 1   | 1     | 2101 | A    |
| 1   | 1     | 2108 | A    |
| 1   | 1     | 2110 | G    |
| 1   | 1     | 2111 | U    |
| 1   | 1     | 2113 | U    |
| 1   | 1     | 2115 | G    |
| 1   | 1     | 2116 | G    |
| 1   | 1     | 2117 | A    |
| 1   | 1     | 2118 | U    |
| 1   | 1     | 2121 | G    |
| 1   | 1     | 2122 | U    |
| 1   | 1     | 2124 | G    |
| 1   | 1     | 2125 | G    |
| 1   | 1     | 2126 | A    |
| 1   | 1     | 2127 | G    |
| 1   | 1     | 2128 | G    |
| 1   | 1     | 2131 | U    |
| 1   | 1     | 2132 | U    |
| 1   | 1     | 2133 | G    |
| 1   | 1     | 2134 | A    |
| 1   | 1     | 2139 | U    |
| 1   | 1     | 2141 | G    |
| 1   | 1     | 2146 | C    |
| 1   | 1     | 2147 | A    |
| 1   | 1     | 2154 | A    |
| 1   | 1     | 2157 | G    |
| 1   | 1     | 2158 | A    |
| 1   | 1     | 2159 | G    |
| 1   | 1     | 2162 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2163 | A    |
| 1   | 1     | 2164 | C    |
| 1   | 1     | 2165 | C    |
| 1   | 1     | 2169 | A    |
| 1   | 1     | 2171 | A    |
| 1   | 1     | 2172 | U    |
| 1   | 1     | 2178 | C    |
| 1   | 1     | 2182 | U    |
| 1   | 1     | 2183 | A    |
| 1   | 1     | 2185 | U    |
| 1   | 1     | 2188 | U    |
| 1   | 1     | 2190 | G    |
| 1   | 1     | 2194 | U    |
| 1   | 1     | 2197 | U    |
| 1   | 1     | 2198 | A    |
| 1   | 1     | 2203 | U    |
| 1   | 1     | 2204 | G    |
| 1   | 1     | 2211 | A    |
| 1   | 1     | 2212 | A    |
| 1   | 1     | 2213 | U    |
| 1   | 1     | 2225 | A    |
| 1   | 1     | 2226 | C    |
| 1   | 1     | 2229 | U    |
| 1   | 1     | 2238 | G    |
| 1   | 1     | 2239 | G    |
| 1   | 1     | 2245 | U    |
| 1   | 1     | 2246 | G    |
| 1   | 1     | 2250 | G    |
| 1   | 1     | 2251 | OMG  |
| 1   | 1     | 2252 | G    |
| 1   | 1     | 2268 | A    |
| 1   | 1     | 2278 | A    |
| 1   | 1     | 2283 | C    |
| 1   | 1     | 2287 | A    |
| 1   | 1     | 2294 | G    |
| 1   | 1     | 2297 | A    |
| 1   | 1     | 2305 | U    |
| 1   | 1     | 2308 | G    |
| 1   | 1     | 2309 | A    |
| 1   | 1     | 2315 | G    |
| 1   | 1     | 2322 | A    |
| 1   | 1     | 2325 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2327 | A    |
| 1   | 1     | 2333 | A    |
| 1   | 1     | 2335 | A    |
| 1   | 1     | 2336 | A    |
| 1   | 1     | 2347 | C    |
| 1   | 1     | 2350 | C    |
| 1   | 1     | 2361 | G    |
| 1   | 1     | 2372 | U    |
| 1   | 1     | 2376 | A    |
| 1   | 1     | 2383 | G    |
| 1   | 1     | 2385 | C    |
| 1   | 1     | 2402 | U    |
| 1   | 1     | 2403 | C    |
| 1   | 1     | 2406 | A    |
| 1   | 1     | 2410 | G    |
| 1   | 1     | 2423 | U    |
| 1   | 1     | 2424 | C    |
| 1   | 1     | 2425 | A    |
| 1   | 1     | 2426 | A    |
| 1   | 1     | 2429 | G    |
| 1   | 1     | 2430 | A    |
| 1   | 1     | 2431 | U    |
| 1   | 1     | 2435 | A    |
| 1   | 1     | 2441 | U    |
| 1   | 1     | 2445 | 2MG  |
| 1   | 1     | 2448 | A    |
| 1   | 1     | 2470 | G    |
| 1   | 1     | 2474 | U    |
| 1   | 1     | 2476 | A    |
| 1   | 1     | 2478 | A    |
| 1   | 1     | 2491 | U    |
| 1   | 1     | 2502 | G    |
| 1   | 1     | 2504 | PSU  |
| 1   | 1     | 2505 | G    |
| 1   | 1     | 2512 | C    |
| 1   | 1     | 2513 | A    |
| 1   | 1     | 2518 | A    |
| 1   | 1     | 2520 | C    |
| 1   | 1     | 2525 | G    |
| 1   | 1     | 2529 | G    |
| 1   | 1     | 2535 | G    |
| 1   | 1     | 2547 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2552 | OMU  |
| 1   | 1     | 2554 | U    |
| 1   | 1     | 2566 | A    |
| 1   | 1     | 2567 | G    |
| 1   | 1     | 2573 | C    |
| 1   | 1     | 2574 | G    |
| 1   | 1     | 2585 | U    |
| 1   | 1     | 2586 | U    |
| 1   | 1     | 2603 | G    |
| 1   | 1     | 2609 | U    |
| 1   | 1     | 2610 | C    |
| 1   | 1     | 2613 | U    |
| 1   | 1     | 2629 | U    |
| 1   | 1     | 2630 | G    |
| 1   | 1     | 2663 | G    |
| 1   | 1     | 2671 | G    |
| 1   | 1     | 2682 | A    |
| 1   | 1     | 2689 | U    |
| 1   | 1     | 2690 | U    |
| 1   | 1     | 2714 | G    |
| 1   | 1     | 2726 | A    |
| 1   | 1     | 2744 | G    |
| 1   | 1     | 2748 | A    |
| 1   | 1     | 2757 | A    |
| 1   | 1     | 2762 | C    |
| 1   | 1     | 2777 | G    |
| 1   | 1     | 2778 | A    |
| 1   | 1     | 2791 | G    |
| 1   | 1     | 2793 | C    |
| 1   | 1     | 2796 | U    |
| 1   | 1     | 2797 | U    |
| 1   | 1     | 2798 | U    |
| 1   | 1     | 2799 | A    |
| 1   | 1     | 2801 | G    |
| 1   | 1     | 2818 | U    |
| 1   | 1     | 2820 | A    |
| 1   | 1     | 2821 | A    |
| 1   | 1     | 2825 | G    |
| 1   | 1     | 2849 | U    |
| 1   | 1     | 2859 | G    |
| 1   | 1     | 2861 | U    |
| 1   | 1     | 2867 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2872 | A    |
| 1   | 1     | 2879 | A    |
| 1   | 1     | 2880 | C    |
| 1   | 1     | 2883 | A    |
| 1   | 1     | 2884 | U    |
| 1   | 1     | 2885 | G    |
| 1   | 1     | 2891 | U    |
| 1   | 1     | 2902 | C    |
| 2   | 2     | 4    | U    |
| 2   | 2     | 5    | U    |
| 2   | 2     | 6    | G    |
| 2   | 2     | 9    | G    |
| 2   | 2     | 19   | A    |
| 2   | 2     | 22   | G    |
| 2   | 2     | 29   | U    |
| 2   | 2     | 32   | A    |
| 2   | 2     | 39   | G    |
| 2   | 2     | 47   | C    |
| 2   | 2     | 48   | C    |
| 2   | 2     | 50   | A    |
| 2   | 2     | 51   | A    |
| 2   | 2     | 52   | C    |
| 2   | 2     | 54   | C    |
| 2   | 2     | 69   | G    |
| 2   | 2     | 70   | U    |
| 2   | 2     | 71   | A    |
| 2   | 2     | 72   | A    |
| 2   | 2     | 74   | A    |
| 2   | 2     | 76   | G    |
| 2   | 2     | 81   | A    |
| 2   | 2     | 82   | G    |
| 2   | 2     | 83   | C    |
| 2   | 2     | 84   | U    |
| 2   | 2     | 87   | C    |
| 2   | 2     | 90   | C    |
| 2   | 2     | 94   | G    |
| 2   | 2     | 95   | C    |
| 2   | 2     | 96   | U    |
| 2   | 2     | 108  | G    |
| 2   | 2     | 120  | A    |
| 2   | 2     | 121  | U    |
| 2   | 2     | 131  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 141 | G    |
| 2   | 2     | 144 | G    |
| 2   | 2     | 148 | G    |
| 2   | 2     | 149 | A    |
| 2   | 2     | 160 | A    |
| 2   | 2     | 164 | G    |
| 2   | 2     | 173 | U    |
| 2   | 2     | 181 | A    |
| 2   | 2     | 182 | A    |
| 2   | 2     | 196 | A    |
| 2   | 2     | 197 | A    |
| 2   | 2     | 198 | G    |
| 2   | 2     | 204 | G    |
| 2   | 2     | 208 | U    |
| 2   | 2     | 209 | U    |
| 2   | 2     | 210 | C    |
| 2   | 2     | 211 | G    |
| 2   | 2     | 212 | G    |
| 2   | 2     | 216 | U    |
| 2   | 2     | 226 | G    |
| 2   | 2     | 245 | U    |
| 2   | 2     | 247 | G    |
| 2   | 2     | 251 | G    |
| 2   | 2     | 258 | G    |
| 2   | 2     | 262 | A    |
| 2   | 2     | 266 | G    |
| 2   | 2     | 267 | C    |
| 2   | 2     | 279 | A    |
| 2   | 2     | 289 | G    |
| 2   | 2     | 306 | A    |
| 2   | 2     | 316 | C    |
| 2   | 2     | 321 | A    |
| 2   | 2     | 328 | C    |
| 2   | 2     | 329 | A    |
| 2   | 2     | 332 | G    |
| 2   | 2     | 340 | U    |
| 2   | 2     | 347 | G    |
| 2   | 2     | 352 | C    |
| 2   | 2     | 354 | G    |
| 2   | 2     | 367 | U    |
| 2   | 2     | 372 | C    |
| 2   | 2     | 373 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 376 | G    |
| 2   | 2     | 384 | G    |
| 2   | 2     | 388 | G    |
| 2   | 2     | 389 | A    |
| 2   | 2     | 392 | C    |
| 2   | 2     | 397 | A    |
| 2   | 2     | 406 | G    |
| 2   | 2     | 412 | A    |
| 2   | 2     | 413 | G    |
| 2   | 2     | 414 | A    |
| 2   | 2     | 421 | U    |
| 2   | 2     | 422 | C    |
| 2   | 2     | 424 | G    |
| 2   | 2     | 429 | U    |
| 2   | 2     | 446 | G    |
| 2   | 2     | 451 | A    |
| 2   | 2     | 457 | G    |
| 2   | 2     | 458 | U    |
| 2   | 2     | 460 | A    |
| 2   | 2     | 463 | U    |
| 2   | 2     | 464 | U    |
| 2   | 2     | 467 | U    |
| 2   | 2     | 468 | A    |
| 2   | 2     | 469 | C    |
| 2   | 2     | 478 | A    |
| 2   | 2     | 479 | U    |
| 2   | 2     | 480 | U    |
| 2   | 2     | 481 | G    |
| 2   | 2     | 484 | G    |
| 2   | 2     | 485 | U    |
| 2   | 2     | 486 | U    |
| 2   | 2     | 495 | A    |
| 2   | 2     | 511 | C    |
| 2   | 2     | 516 | PSU  |
| 2   | 2     | 517 | G    |
| 2   | 2     | 518 | C    |
| 2   | 2     | 521 | G    |
| 2   | 2     | 526 | C    |
| 2   | 2     | 531 | U    |
| 2   | 2     | 532 | A    |
| 2   | 2     | 533 | A    |
| 2   | 2     | 547 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 559 | A    |
| 2   | 2     | 568 | G    |
| 2   | 2     | 572 | A    |
| 2   | 2     | 573 | A    |
| 2   | 2     | 576 | C    |
| 2   | 2     | 577 | G    |
| 2   | 2     | 579 | A    |
| 2   | 2     | 587 | G    |
| 2   | 2     | 588 | G    |
| 2   | 2     | 596 | A    |
| 2   | 2     | 628 | G    |
| 2   | 2     | 633 | G    |
| 2   | 2     | 642 | A    |
| 2   | 2     | 649 | A    |
| 2   | 2     | 650 | G    |
| 2   | 2     | 653 | U    |
| 2   | 2     | 656 | G    |
| 2   | 2     | 665 | A    |
| 2   | 2     | 687 | A    |
| 2   | 2     | 700 | G    |
| 2   | 2     | 702 | A    |
| 2   | 2     | 723 | U    |
| 2   | 2     | 724 | G    |
| 2   | 2     | 731 | G    |
| 2   | 2     | 734 | G    |
| 2   | 2     | 747 | A    |
| 2   | 2     | 748 | G    |
| 2   | 2     | 755 | G    |
| 2   | 2     | 777 | A    |
| 2   | 2     | 793 | U    |
| 2   | 2     | 794 | A    |
| 2   | 2     | 815 | A    |
| 2   | 2     | 817 | C    |
| 2   | 2     | 828 | U    |
| 2   | 2     | 841 | C    |
| 2   | 2     | 844 | G    |
| 2   | 2     | 845 | A    |
| 2   | 2     | 849 | G    |
| 2   | 2     | 874 | G    |
| 2   | 2     | 887 | G    |
| 2   | 2     | 902 | G    |
| 2   | 2     | 914 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 916  | U    |
| 2   | 2     | 926  | G    |
| 2   | 2     | 928  | G    |
| 2   | 2     | 934  | C    |
| 2   | 2     | 935  | A    |
| 2   | 2     | 936  | C    |
| 2   | 2     | 960  | U    |
| 2   | 2     | 961  | U    |
| 2   | 2     | 966  | 2MG  |
| 2   | 2     | 967  | 5MC  |
| 2   | 2     | 969  | A    |
| 2   | 2     | 972  | C    |
| 2   | 2     | 975  | A    |
| 2   | 2     | 976  | G    |
| 2   | 2     | 977  | A    |
| 2   | 2     | 987  | G    |
| 2   | 2     | 991  | U    |
| 2   | 2     | 992  | U    |
| 2   | 2     | 993  | G    |
| 2   | 2     | 996  | A    |
| 2   | 2     | 999  | C    |
| 2   | 2     | 1004 | A    |
| 2   | 2     | 1005 | A    |
| 2   | 2     | 1008 | U    |
| 2   | 2     | 1009 | U    |
| 2   | 2     | 1017 | U    |
| 2   | 2     | 1018 | G    |
| 2   | 2     | 1021 | A    |
| 2   | 2     | 1024 | G    |
| 2   | 2     | 1026 | G    |
| 2   | 2     | 1028 | C    |
| 2   | 2     | 1030 | U    |
| 2   | 2     | 1031 | C    |
| 2   | 2     | 1037 | C    |
| 2   | 2     | 1042 | A    |
| 2   | 2     | 1043 | G    |
| 2   | 2     | 1044 | A    |
| 2   | 2     | 1046 | A    |
| 2   | 2     | 1065 | U    |
| 2   | 2     | 1085 | U    |
| 2   | 2     | 1086 | U    |
| 2   | 2     | 1092 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 1094 | G    |
| 2   | 2     | 1095 | U    |
| 2   | 2     | 1099 | G    |
| 2   | 2     | 1101 | A    |
| 2   | 2     | 1124 | G    |
| 2   | 2     | 1133 | G    |
| 2   | 2     | 1135 | U    |
| 2   | 2     | 1136 | C    |
| 2   | 2     | 1137 | C    |
| 2   | 2     | 1139 | G    |
| 2   | 2     | 1140 | C    |
| 2   | 2     | 1141 | C    |
| 2   | 2     | 1142 | G    |
| 2   | 2     | 1143 | G    |
| 2   | 2     | 1145 | A    |
| 2   | 2     | 1146 | A    |
| 2   | 2     | 1151 | A    |
| 2   | 2     | 1152 | A    |
| 2   | 2     | 1158 | C    |
| 2   | 2     | 1159 | U    |
| 2   | 2     | 1167 | A    |
| 2   | 2     | 1171 | A    |
| 2   | 2     | 1174 | G    |
| 2   | 2     | 1175 | G    |
| 2   | 2     | 1176 | A    |
| 2   | 2     | 1184 | G    |
| 2   | 2     | 1187 | G    |
| 2   | 2     | 1196 | A    |
| 2   | 2     | 1197 | A    |
| 2   | 2     | 1211 | U    |
| 2   | 2     | 1212 | U    |
| 2   | 2     | 1213 | A    |
| 2   | 2     | 1214 | C    |
| 2   | 2     | 1215 | G    |
| 2   | 2     | 1227 | A    |
| 2   | 2     | 1238 | A    |
| 2   | 2     | 1239 | A    |
| 2   | 2     | 1242 | G    |
| 2   | 2     | 1257 | A    |
| 2   | 2     | 1260 | G    |
| 2   | 2     | 1275 | A    |
| 2   | 2     | 1276 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 1277 | C    |
| 2   | 2     | 1278 | G    |
| 2   | 2     | 1279 | G    |
| 2   | 2     | 1280 | A    |
| 2   | 2     | 1285 | A    |
| 2   | 2     | 1286 | U    |
| 2   | 2     | 1287 | A    |
| 2   | 2     | 1299 | A    |
| 2   | 2     | 1300 | G    |
| 2   | 2     | 1302 | C    |
| 2   | 2     | 1305 | G    |
| 2   | 2     | 1311 | A    |
| 2   | 2     | 1312 | G    |
| 2   | 2     | 1317 | C    |
| 2   | 2     | 1320 | C    |
| 2   | 2     | 1323 | G    |
| 2   | 2     | 1329 | A    |
| 2   | 2     | 1332 | A    |
| 2   | 2     | 1334 | G    |
| 2   | 2     | 1338 | G    |
| 2   | 2     | 1340 | A    |
| 2   | 2     | 1346 | A    |
| 2   | 2     | 1353 | G    |
| 2   | 2     | 1363 | A    |
| 2   | 2     | 1370 | G    |
| 2   | 2     | 1378 | C    |
| 2   | 2     | 1379 | G    |
| 2   | 2     | 1381 | U    |
| 2   | 2     | 1383 | C    |
| 2   | 2     | 1396 | A    |
| 2   | 2     | 1397 | C    |
| 2   | 2     | 1404 | C    |
| 2   | 2     | 1408 | A    |
| 2   | 2     | 1419 | G    |
| 2   | 2     | 1429 | A    |
| 2   | 2     | 1441 | A    |
| 2   | 2     | 1446 | A    |
| 2   | 2     | 1447 | A    |
| 2   | 2     | 1448 | C    |
| 2   | 2     | 1452 | C    |
| 2   | 2     | 1453 | G    |
| 2   | 2     | 1487 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 1493 | A    |
| 2   | 2     | 1494 | G    |
| 2   | 2     | 1497 | G    |
| 2   | 2     | 1503 | A    |
| 2   | 2     | 1506 | U    |
| 2   | 2     | 1517 | G    |
| 2   | 2     | 1529 | G    |
| 2   | 2     | 1530 | G    |
| 2   | 2     | 1534 | A    |
| 3   | 3     | 2    | G    |
| 3   | 3     | 13   | G    |
| 3   | 3     | 16   | G    |
| 3   | 3     | 17   | C    |
| 3   | 3     | 35   | C    |
| 3   | 3     | 36   | C    |
| 3   | 3     | 45   | A    |
| 3   | 3     | 56   | G    |
| 3   | 3     | 64   | G    |
| 3   | 3     | 66   | A    |
| 3   | 3     | 88   | C    |
| 3   | 3     | 89   | U    |
| 3   | 3     | 90   | C    |
| 3   | 3     | 99   | A    |
| 3   | 3     | 109  | A    |
| 4   | 4     | 15   | A    |
| 5   | 5     | 5    | G    |
| 5   | 5     | 8    | 4SU  |
| 5   | 5     | 13   | A    |
| 5   | 5     | 15   | C    |
| 5   | 5     | 16   | C    |
| 5   | 5     | 17   | U    |
| 5   | 5     | 18   | G    |
| 5   | 5     | 19   | G    |
| 5   | 5     | 20   | H2U  |
| 5   | 5     | 21   | A    |
| 5   | 5     | 22   | G    |
| 5   | 5     | 25   | C    |
| 5   | 5     | 31   | G    |
| 5   | 5     | 37   | A    |
| 5   | 5     | 47   | U    |
| 5   | 5     | 48   | C    |
| 5   | 5     | 49   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 5     | 55  | PSU  |
| 5   | 5     | 57  | A    |
| 5   | 5     | 59  | A    |
| 5   | 5     | 69  | C    |
| 5   | 5     | 74  | C    |
| 5   | 5     | 75  | C    |

All (127) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 33   | C    |
| 1   | 1     | 62   | U    |
| 1   | 1     | 70   | G    |
| 1   | 1     | 71   | A    |
| 1   | 1     | 101  | A    |
| 1   | 1     | 125  | A    |
| 1   | 1     | 138  | U    |
| 1   | 1     | 140  | C    |
| 1   | 1     | 196  | A    |
| 1   | 1     | 199  | A    |
| 1   | 1     | 271  | G    |
| 1   | 1     | 310  | A    |
| 1   | 1     | 404  | A    |
| 1   | 1     | 446  | G    |
| 1   | 1     | 503  | A    |
| 1   | 1     | 532  | A    |
| 1   | 1     | 545  | U    |
| 1   | 1     | 546  | U    |
| 1   | 1     | 685  | A    |
| 1   | 1     | 748  | G    |
| 1   | 1     | 764  | A    |
| 1   | 1     | 776  | G    |
| 1   | 1     | 784  | G    |
| 1   | 1     | 883  | G    |
| 1   | 1     | 884  | U    |
| 1   | 1     | 892  | A    |
| 1   | 1     | 894  | U    |
| 1   | 1     | 896  | A    |
| 1   | 1     | 984  | A    |
| 1   | 1     | 1045 | C    |
| 1   | 1     | 1060 | U    |
| 1   | 1     | 1064 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1067 | A    |
| 1   | 1     | 1069 | A    |
| 1   | 1     | 1070 | A    |
| 1   | 1     | 1111 | A    |
| 1   | 1     | 1128 | G    |
| 1   | 1     | 1173 | U    |
| 1   | 1     | 1174 | U    |
| 1   | 1     | 1300 | G    |
| 1   | 1     | 1320 | C    |
| 1   | 1     | 1344 | U    |
| 1   | 1     | 1379 | U    |
| 1   | 1     | 1395 | A    |
| 1   | 1     | 1405 | U    |
| 1   | 1     | 1407 | G    |
| 1   | 1     | 1408 | G    |
| 1   | 1     | 1490 | A    |
| 1   | 1     | 1509 | A    |
| 1   | 1     | 1584 | U    |
| 1   | 1     | 1596 | A    |
| 1   | 1     | 1608 | A    |
| 1   | 1     | 1647 | U    |
| 1   | 1     | 1784 | A    |
| 1   | 1     | 1912 | A    |
| 1   | 1     | 1913 | A    |
| 1   | 1     | 1918 | A    |
| 1   | 1     | 1962 | 5MC  |
| 1   | 1     | 2062 | A    |
| 1   | 1     | 2146 | C    |
| 1   | 1     | 2162 | G    |
| 1   | 1     | 2193 | G    |
| 1   | 1     | 2197 | U    |
| 1   | 1     | 2198 | A    |
| 1   | 1     | 2210 | U    |
| 1   | 1     | 2211 | A    |
| 1   | 1     | 2212 | A    |
| 1   | 1     | 2225 | A    |
| 1   | 1     | 2250 | G    |
| 1   | 1     | 2296 | U    |
| 1   | 1     | 2308 | G    |
| 1   | 1     | 2425 | A    |
| 1   | 1     | 2447 | G    |
| 1   | 1     | 2573 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2585 | U    |
| 1   | 1     | 2602 | A    |
| 1   | 1     | 2610 | C    |
| 1   | 1     | 2756 | U    |
| 1   | 1     | 2797 | U    |
| 1   | 1     | 2798 | U    |
| 1   | 1     | 2873 | A    |
| 2   | 2     | 5    | U    |
| 2   | 2     | 70   | U    |
| 2   | 2     | 121  | U    |
| 2   | 2     | 147  | G    |
| 2   | 2     | 148  | G    |
| 2   | 2     | 181  | A    |
| 2   | 2     | 183  | C    |
| 2   | 2     | 197  | A    |
| 2   | 2     | 209  | U    |
| 2   | 2     | 421  | U    |
| 2   | 2     | 428  | G    |
| 2   | 2     | 481  | G    |
| 2   | 2     | 496  | A    |
| 2   | 2     | 587  | G    |
| 2   | 2     | 641  | U    |
| 2   | 2     | 701  | U    |
| 2   | 2     | 793  | U    |
| 2   | 2     | 873  | A    |
| 2   | 2     | 961  | U    |
| 2   | 2     | 966  | 2MG  |
| 2   | 2     | 967  | 5MC  |
| 2   | 2     | 974  | A    |
| 2   | 2     | 991  | U    |
| 2   | 2     | 992  | U    |
| 2   | 2     | 1129 | C    |
| 2   | 2     | 1145 | A    |
| 2   | 2     | 1196 | A    |
| 2   | 2     | 1211 | U    |
| 2   | 2     | 1213 | A    |
| 2   | 2     | 1214 | C    |
| 2   | 2     | 1277 | C    |
| 2   | 2     | 1299 | A    |
| 2   | 2     | 1319 | A    |
| 2   | 2     | 1363 | A    |
| 2   | 2     | 1396 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 1447 | A    |
| 2   | 2     | 1516 | 2MG  |
| 5   | 5     | 14   | G    |
| 5   | 5     | 15   | C    |
| 5   | 5     | 16   | C    |
| 5   | 5     | 17   | U    |
| 5   | 5     | 18   | G    |
| 5   | 5     | 20   | H2U  |
| 5   | 5     | 21   | A    |
| 5   | 5     | 47   | U    |
| 5   | 5     | 60   | U    |

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

41 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 |
| 1   | 6MZ  | 1     | 1618 | 1    | 17,25,26     | 0.89 | 1 (5%)   | 15,36,39    | 1.89 | 4 (26%)  |
| 1   | 2MG  | 1     | 1835 | 1    | 18,26,27     | 1.28 | 1 (5%)   | 21,38,41    | 2.85 | 6 (28%)  |
| 1   | PSU  | 1     | 1911 | 1    | 15,21,22     | 1.95 | 4 (26%)  | 16,30,33    | 2.41 | 6 (37%)  |
| 1   | 3TD  | 1     | 1915 | 1    | 15,22,23     | 1.20 | 1 (6%)   | 17,32,35    | 2.27 | 7 (41%)  |
| 1   | PSU  | 1     | 1917 | 1    | 15,21,22     | 1.98 | 4 (26%)  | 16,30,33    | 2.45 | 4 (25%)  |
| 1   | 5MU  | 1     | 1939 | 1    | 13,22,23     | 1.13 | 2 (15%)  | 16,32,35    | 2.27 | 2 (12%)  |
| 1   | 5MC  | 1     | 1962 | 1    | 14,22,23     | 1.57 | 1 (7%)   | 17,32,35    | 1.16 | 1 (5%)   |
| 1   | 6MZ  | 1     | 2030 | 1    | 17,25,26     | 0.96 | 1 (5%)   | 15,36,39    | 2.21 | 4 (26%)  |
| 1   | G7M  | 1     | 2069 | 1    | 18,26,27     | 1.68 | 2 (11%)  | 21,39,42    | 3.78 | 10 (47%) |
| 1   | OMG  | 1     | 2251 | 1,5  | 18,26,27     | 0.98 | 2 (11%)  | 21,38,41    | 2.06 | 6 (28%)  |
| 1   | 2MG  | 1     | 2445 | 1    | 18,26,27     | 1.38 | 1 (5%)   | 21,38,41    | 2.79 | 6 (28%)  |
| 1   | PSU  | 1     | 2457 | 1,59 | 15,21,22     | 3.24 | 4 (26%)  | 16,30,33    | 3.63 | 7 (43%)  |
| 1   | OMC  | 1     | 2498 | 1,59 | 15,22,23     | 1.11 | 1 (6%)   | 20,31,34    | 1.70 | 3 (15%)  |
| 1   | 2MA  | 1     | 2503 | 1,59 | 17,25,26     | 1.45 | 3 (17%)  | 18,37,40    | 2.94 | 6 (33%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | PSU  | 1     | 2504 | 1    | 15,21,22     | 3.36 | 4 (26%)  | 16,30,33    | 3.60 | 8 (50%)  |
| 1   | OMU  | 1     | 2552 | 1,59 | 14,22,23     | 1.02 | 1 (7%)   | 19,31,34    | 2.32 | 2 (10%)  |
| 1   | PSU  | 1     | 2580 | 1    | 15,21,22     | 2.91 | 4 (26%)  | 16,30,33    | 3.79 | 7 (43%)  |
| 1   | PSU  | 1     | 2605 | 1    | 15,21,22     | 3.43 | 4 (26%)  | 16,30,33    | 3.79 | 8 (50%)  |
| 1   | 1MG  | 1     | 745  | 1    | 17,26,27     | 1.50 | 2 (11%)  | 19,39,42    | 1.87 | 5 (26%)  |
| 1   | PSU  | 1     | 746  | 1,59 | 15,21,22     | 3.42 | 3 (20%)  | 16,30,33    | 3.95 | 6 (37%)  |
| 1   | 5MU  | 1     | 747  | 1    | 13,22,23     | 1.65 | 2 (15%)  | 16,32,35    | 4.02 | 4 (25%)  |
| 1   | PSU  | 1     | 955  | 1    | 15,21,22     | 3.20 | 4 (26%)  | 16,30,33    | 3.75 | 8 (50%)  |
| 2   | 2MG  | 2     | 1207 | 2    | 18,26,27     | 1.38 | 2 (11%)  | 21,38,41    | 2.81 | 10 (47%) |
| 2   | 4OC  | 2     | 1402 | 2    | 15,23,24     | 1.33 | 2 (13%)  | 21,32,35    | 1.89 | 5 (23%)  |
| 2   | 5MC  | 2     | 1407 | 2    | 14,22,23     | 0.62 | 0        | 17,32,35    | 0.88 | 0        |
| 2   | UR3  | 2     | 1498 | 2    | 13,22,23     | 1.48 | 2 (15%)  | 18,32,35    | 1.13 | 1 (5%)   |
| 2   | 2MG  | 2     | 1516 | 2    | 18,26,27     | 1.31 | 1 (5%)   | 21,38,41    | 2.82 | 7 (33%)  |
| 2   | MA6  | 2     | 1518 | 2    | 18,26,27     | 0.53 | 0        | 15,38,41    | 1.53 | 3 (20%)  |
| 2   | MA6  | 2     | 1519 | 2    | 18,26,27     | 0.56 | 0        | 15,38,41    | 1.47 | 3 (20%)  |
| 2   | PSU  | 2     | 516  | 2,59 | 15,21,22     | 2.68 | 4 (26%)  | 16,30,33    | 3.74 | 6 (37%)  |
| 2   | 7MG  | 2     | 527  | 2    | 20,26,27     | 1.27 | 1 (5%)   | 23,39,42    | 3.41 | 7 (30%)  |
| 2   | 2MG  | 2     | 966  | 2    | 18,26,27     | 1.32 | 1 (5%)   | 21,38,41    | 3.18 | 8 (38%)  |
| 2   | 5MC  | 2     | 967  | 2    | 14,22,23     | 1.45 | 1 (7%)   | 17,32,35    | 1.61 | 2 (11%)  |
| 5   | H2U  | 5     | 20   | 5    | 17,21,22     | 0.72 | 0        | 23,30,33    | 1.84 | 4 (17%)  |
| 5   | 4OC  | 5     | 32   | 5    | 15,23,24     | 0.74 | 0        | 21,32,35    | 1.82 | 5 (23%)  |
| 5   | 5MU  | 5     | 54   | 5    | 13,22,23     | 1.41 | 2 (15%)  | 16,32,35    | 4.12 | 5 (31%)  |
| 5   | PSU  | 5     | 55   | 5    | 15,21,22     | 3.03 | 4 (26%)  | 16,30,33    | 3.58 | 5 (31%)  |
| 5   | 8AN  | 5     | 76   | 60,5 | 18,24,25     | 0.62 | 0        | 10,35,38    | 0.38 | 0        |
| 5   | 4SU  | 5     | 8    | 5    | 12,21,22     | 0.72 | 0        | 15,30,33    | 1.20 | 2 (13%)  |
| 7   | MEQ  | 7     | 252  | 7    | 7,9,10       | 0.46 | 0        | 8,10,12     | 1.63 | 2 (25%)  |
| 49  | 0TD  | q     | 89   | 49   | 4,9,10       | 4.31 | 3 (75%)  | 4,11,13     | 5.61 | 4 (100%) |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | 6MZ  | 1     | 1618 | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | 2MG  | 1     | 1835 | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | PSU  | 1     | 1911 | 1    | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | 3TD  | 1     | 1915 | 1    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | PSU  | 1     | 1917 | 1    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 5MU  | 1     | 1939 | 1    | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | 5MC  | 1     | 1962 | 1    | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | 6MZ  | 1     | 2030 | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | G7M  | 1     | 2069 | 1    | -       | 0/3/25/26 | 0/3/3/3 |
| 1   | OMG  | 1     | 2251 | 1,5  | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | 2MG  | 1     | 2445 | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | PSU  | 1     | 2457 | 1,59 | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMC  | 1     | 2498 | 1,59 | -       | 0/5/27/28 | 0/2/2/2 |
| 1   | 2MA  | 1     | 2503 | 1,59 | -       | 0/3/25/26 | 0/3/3/3 |
| 1   | PSU  | 1     | 2504 | 1    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMU  | 1     | 2552 | 1,59 | -       | 0/5/27/28 | 0/2/2/2 |
| 1   | PSU  | 1     | 2580 | 1    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | PSU  | 1     | 2605 | 1    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 1MG  | 1     | 745  | 1    | -       | 0/3/25/26 | 0/3/3/3 |
| 1   | PSU  | 1     | 746  | 1,59 | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 5MU  | 1     | 747  | 1    | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | PSU  | 1     | 955  | 1    | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | 2MG  | 2     | 1207 | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | 4OC  | 2     | 1402 | 2    | -       | 0/7/29/30 | 0/2/2/2 |
| 2   | 5MC  | 2     | 1407 | 2    | -       | 0/3/25/26 | 0/2/2/2 |
| 2   | UR3  | 2     | 1498 | 2    | -       | 0/3/25/26 | 0/2/2/2 |
| 2   | 2MG  | 2     | 1516 | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | MA6  | 2     | 1518 | 2    | -       | 0/7/29/30 | 0/3/3/3 |
| 2   | MA6  | 2     | 1519 | 2    | -       | 0/7/29/30 | 0/3/3/3 |
| 2   | PSU  | 2     | 516  | 2,59 | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | 7MG  | 2     | 527  | 2    | -       | 0/7/37/38 | 0/3/3/3 |
| 2   | 2MG  | 2     | 966  | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | 5MC  | 2     | 967  | 2    | -       | 0/3/25/26 | 0/2/2/2 |
| 5   | H2U  | 5     | 20   | 5    | -       | 0/7/38/39 | 0/2/2/2 |
| 5   | 4OC  | 5     | 32   | 5    | -       | 0/7/29/30 | 0/2/2/2 |
| 5   | 5MU  | 5     | 54   | 5    | -       | 0/3/25/26 | 0/2/2/2 |
| 5   | PSU  | 5     | 55   | 5    | -       | 0/7/25/26 | 0/2/2/2 |
| 5   | 8AN  | 5     | 76   | 60,5 | -       | 0/3/25/26 | 0/3/3/3 |
| 5   | 4SU  | 5     | 8    | 5    | -       | 0/3/25/26 | 0/2/2/2 |
| 7   | MEQ  | 7     | 252  | 7    | -       | 1/7/9/11  | 0/0/0/0 |
| 49  | 0TD  | q     | 89   | 49   | -       | 0/2/12/14 | 0/0/0/0 |

All (75) bond length outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
|-----|-------|-----|------|-------|---|-------------|----------|

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | 1     | 746  | PSU  | C2'-C1' | -12.27 | 1.42        | 1.53     |
| 1   | 1     | 2605 | PSU  | C2'-C1' | -11.94 | 1.42        | 1.53     |
| 1   | 1     | 2504 | PSU  | C2'-C1' | -11.76 | 1.42        | 1.53     |
| 1   | 1     | 2457 | PSU  | C2'-C1' | -11.15 | 1.43        | 1.53     |
| 1   | 1     | 955  | PSU  | C2'-C1' | -10.74 | 1.43        | 1.53     |
| 5   | 5     | 55   | PSU  | C2'-C1' | -10.57 | 1.43        | 1.53     |
| 1   | 1     | 2580 | PSU  | C2'-C1' | -9.76  | 1.44        | 1.53     |
| 2   | 2     | 516  | PSU  | C2'-C1' | -8.82  | 1.45        | 1.53     |
| 49  | q     | 89   | 0TD  | CB-SB   | -7.53  | 1.65        | 1.84     |
| 1   | 1     | 1917 | PSU  | C5-C1'  | -5.73  | 1.47        | 1.52     |
| 1   | 1     | 1962 | 5MC  | C2'-C1' | -5.19  | 1.45        | 1.53     |
| 1   | 1     | 2069 | G7M  | C2'-C1' | -5.16  | 1.45        | 1.53     |
| 1   | 1     | 1911 | PSU  | C5-C1'  | -5.03  | 1.47        | 1.52     |
| 2   | 2     | 967  | 5MC  | C2'-C1' | -4.77  | 1.46        | 1.53     |
| 1   | 1     | 747  | 5MU  | C2'-C1' | -4.73  | 1.46        | 1.53     |
| 1   | 1     | 745  | 1MG  | C2'-C1' | -4.55  | 1.46        | 1.53     |
| 1   | 1     | 1911 | PSU  | C2'-C1' | -3.76  | 1.50        | 1.53     |
| 5   | 5     | 54   | 5MU  | C2'-C1' | -3.67  | 1.47        | 1.53     |
| 1   | 1     | 955  | PSU  | C5-C1'  | -3.56  | 1.49        | 1.52     |
| 49  | q     | 89   | 0TD  | CA-N    | -3.38  | 1.37        | 1.47     |
| 2   | 2     | 1207 | 2MG  | C2'-C1' | -3.37  | 1.48        | 1.53     |
| 1   | 1     | 2504 | PSU  | C5-C1'  | -3.22  | 1.49        | 1.52     |
| 1   | 1     | 2498 | OMC  | C3'-C2' | -3.21  | 1.45        | 1.53     |
| 1   | 1     | 2457 | PSU  | C5-C1'  | -3.19  | 1.49        | 1.52     |
| 1   | 1     | 1915 | 3TD  | C6-C5   | -3.17  | 1.34        | 1.38     |
| 1   | 1     | 2605 | PSU  | C5-C1'  | -3.15  | 1.49        | 1.52     |
| 2   | 2     | 1498 | UR3  | C6-N1   | -3.09  | 1.31        | 1.35     |
| 1   | 1     | 1917 | PSU  | C2'-C1' | -3.06  | 1.50        | 1.53     |
| 1   | 1     | 2580 | PSU  | C6-C5   | -3.02  | 1.34        | 1.38     |
| 1   | 1     | 746  | PSU  | C6-C5   | -3.02  | 1.34        | 1.38     |
| 2   | 2     | 516  | PSU  | C5-C1'  | -2.98  | 1.49        | 1.52     |
| 1   | 1     | 955  | PSU  | C6-C5   | -2.97  | 1.34        | 1.38     |
| 1   | 1     | 2580 | PSU  | C5-C1'  | -2.96  | 1.49        | 1.52     |
| 1   | 1     | 2605 | PSU  | C6-C5   | -2.89  | 1.34        | 1.38     |
| 2   | 2     | 516  | PSU  | C6-C5   | -2.87  | 1.34        | 1.38     |
| 1   | 1     | 2030 | 6MZ  | C2'-C1' | -2.85  | 1.49        | 1.53     |
| 2   | 2     | 1402 | 4OC  | C2-N3   | -2.84  | 1.32        | 1.38     |
| 1   | 1     | 2504 | PSU  | C6-C5   | -2.82  | 1.34        | 1.38     |
| 1   | 1     | 2457 | PSU  | C6-C5   | -2.81  | 1.34        | 1.38     |
| 1   | 1     | 1939 | 5MU  | C2-N3   | -2.79  | 1.32        | 1.38     |
| 2   | 2     | 1498 | UR3  | C2'-C1' | -2.74  | 1.49        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | 1     | 1911 | PSU  | C2-N3   | -2.65 | 1.32        | 1.38     |
| 2   | 2     | 1402 | 4OC  | C6-N1   | -2.62 | 1.32        | 1.35     |
| 5   | 5     | 55   | PSU  | C6-C5   | -2.60 | 1.34        | 1.38     |
| 1   | 1     | 1917 | PSU  | C2-N3   | -2.52 | 1.32        | 1.38     |
| 49  | q     | 89   | 0TD  | CSB-SB  | -2.47 | 1.74        | 1.79     |
| 1   | 1     | 1917 | PSU  | C2-N1   | -2.43 | 1.33        | 1.38     |
| 1   | 1     | 1911 | PSU  | C2-N1   | -2.37 | 1.33        | 1.38     |
| 1   | 1     | 1618 | 6MZ  | C2'-C1' | -2.33 | 1.49        | 1.53     |
| 5   | 5     | 55   | PSU  | C5-C1'  | -2.30 | 1.50        | 1.52     |
| 1   | 1     | 1939 | 5MU  | C2'-C1' | -2.11 | 1.50        | 1.53     |
| 1   | 1     | 2503 | 2MA  | C2'-C3' | -2.10 | 1.47        | 1.53     |
| 1   | 1     | 2251 | OMG  | C5-C4   | 2.04  | 1.45        | 1.40     |
| 1   | 1     | 745  | 1MG  | C6-N1   | 2.05  | 1.41        | 1.38     |
| 2   | 2     | 1207 | 2MG  | C6-C5   | 2.33  | 1.46        | 1.41     |
| 1   | 1     | 2503 | 2MA  | C6-N1   | 2.37  | 1.39        | 1.34     |
| 2   | 2     | 527  | 7MG  | C6-C5   | 2.43  | 1.44        | 1.41     |
| 1   | 1     | 2251 | OMG  | C6-C5   | 2.51  | 1.46        | 1.41     |
| 1   | 1     | 2580 | PSU  | C4-N3   | 2.54  | 1.37        | 1.33     |
| 2   | 2     | 516  | PSU  | C4-N3   | 2.72  | 1.37        | 1.33     |
| 1   | 1     | 2504 | PSU  | C4-N3   | 2.73  | 1.38        | 1.33     |
| 1   | 1     | 955  | PSU  | C4-N3   | 2.74  | 1.38        | 1.33     |
| 1   | 1     | 2457 | PSU  | C4-N3   | 2.77  | 1.38        | 1.33     |
| 1   | 1     | 2605 | PSU  | C4-N3   | 2.80  | 1.38        | 1.33     |
| 1   | 1     | 746  | PSU  | C4-N3   | 2.80  | 1.38        | 1.33     |
| 5   | 5     | 55   | PSU  | C4-N3   | 2.91  | 1.38        | 1.33     |
| 1   | 1     | 2552 | OMU  | C4-N3   | 2.94  | 1.38        | 1.33     |
| 1   | 1     | 747  | 5MU  | C4-N3   | 3.17  | 1.38        | 1.33     |
| 5   | 5     | 54   | 5MU  | C4-N3   | 3.21  | 1.38        | 1.33     |
| 1   | 1     | 2069 | G7M  | C6-N1   | 3.31  | 1.39        | 1.33     |
| 1   | 1     | 2503 | 2MA  | C2-N1   | 4.08  | 1.41        | 1.34     |
| 1   | 1     | 1835 | 2MG  | C6-N1   | 4.63  | 1.41        | 1.33     |
| 1   | 1     | 2445 | 2MG  | C6-N1   | 4.68  | 1.41        | 1.33     |
| 2   | 2     | 1516 | 2MG  | C6-N1   | 4.71  | 1.41        | 1.33     |
| 2   | 2     | 966  | 2MG  | C6-N1   | 4.86  | 1.41        | 1.33     |

All (199) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 5   | 5     | 54   | 5MU  | C5-C4-N3    | -10.79 | 116.29      | 125.35   |
| 1   | 1     | 747  | 5MU  | C5-C4-N3    | -10.76 | 116.32      | 125.35   |
| 2   | 2     | 527  | 7MG  | C5-C4-N3    | -9.67  | 116.89      | 126.74   |
| 1   | 1     | 2069 | G7M  | C4'-O4'-C1' | -9.44  | 99.63       | 109.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | 2     | 1516 | 2MG  | C5-C6-N1    | -9.07 | 111.67      | 123.52   |
| 1   | 1     | 1835 | 2MG  | C5-C6-N1    | -9.04 | 111.71      | 123.52   |
| 2   | 2     | 966  | 2MG  | C5-C6-N1    | -9.02 | 111.73      | 123.52   |
| 1   | 1     | 2445 | 2MG  | C5-C6-N1    | -8.99 | 111.77      | 123.52   |
| 49  | q     | 89   | 0TD  | CB-CA-N     | -8.37 | 93.08       | 109.83   |
| 1   | 1     | 2069 | G7M  | C5-C6-N1    | -7.92 | 113.17      | 123.52   |
| 1   | 1     | 2503 | 2MA  | C4'-O4'-C1' | -7.77 | 101.40      | 109.64   |
| 1   | 1     | 1939 | 5MU  | C5-C4-N3    | -6.47 | 119.92      | 125.35   |
| 2   | 2     | 527  | 7MG  | C5-C6-N1    | -5.18 | 115.68      | 123.39   |
| 2   | 2     | 1207 | 2MG  | C6-C5-C4    | -5.15 | 114.97      | 120.86   |
| 1   | 1     | 1917 | PSU  | C5-C1'-C2'  | -5.11 | 106.75      | 115.44   |
| 1   | 1     | 2030 | 6MZ  | C4'-O4'-C1' | -4.95 | 104.40      | 109.64   |
| 1   | 1     | 1915 | 3TD  | C5-C1'-C2'  | -4.87 | 107.16      | 115.44   |
| 2   | 2     | 1207 | 2MG  | C1'-N9-C4   | -4.84 | 121.41      | 126.81   |
| 1   | 1     | 955  | PSU  | C4'-O4'-C1' | -4.34 | 105.08      | 109.54   |
| 1   | 1     | 2605 | PSU  | C4'-O4'-C1' | -4.34 | 105.08      | 109.54   |
| 1   | 1     | 1911 | PSU  | C5-C1'-C2'  | -4.18 | 108.33      | 115.44   |
| 1   | 1     | 1915 | 3TD  | C5'-C4'-C3' | -4.13 | 99.24       | 115.20   |
| 2   | 2     | 966  | 2MG  | C4'-O4'-C1' | -4.09 | 105.31      | 109.64   |
| 2   | 2     | 1207 | 2MG  | CM2-N2-C2   | -3.93 | 118.62      | 123.03   |
| 1   | 1     | 1915 | 3TD  | O2'-C2'-C1' | -3.77 | 103.72      | 111.93   |
| 2   | 2     | 1402 | 4OC  | CM4-N4-C4   | -3.75 | 119.71      | 122.87   |
| 1   | 1     | 2251 | OMG  | C6-C5-C4    | -3.70 | 116.63      | 120.86   |
| 1   | 1     | 2251 | OMG  | C5-C6-N1    | -3.69 | 118.70      | 123.52   |
| 1   | 1     | 1911 | PSU  | C5-C6-N1    | -3.62 | 119.33      | 124.38   |
| 1   | 1     | 1917 | PSU  | C5-C6-N1    | -3.54 | 119.44      | 124.38   |
| 1   | 1     | 2251 | OMG  | N3-C2-N1    | -3.49 | 122.81      | 127.56   |
| 2   | 2     | 966  | 2MG  | C2'-C3'-C4' | -3.43 | 95.61       | 102.64   |
| 2   | 2     | 1207 | 2MG  | C5-C6-N1    | -3.30 | 119.21      | 123.52   |
| 1   | 1     | 745  | 1MG  | C5-C6-N1    | -3.19 | 114.17      | 118.35   |
| 1   | 1     | 2069 | G7M  | N3-C2-N1    | -2.92 | 123.58      | 127.56   |
| 2   | 2     | 1207 | 2MG  | O2'-C2'-C1' | -2.91 | 102.52      | 111.61   |
| 1   | 1     | 2605 | PSU  | C2'-C3'-C4' | -2.89 | 96.71       | 102.64   |
| 2   | 2     | 527  | 7MG  | O4'-C4'-C3' | -2.85 | 99.39       | 105.16   |
| 5   | 5     | 8    | 4SU  | C4'-O4'-C1' | -2.81 | 106.66      | 109.64   |
| 1   | 1     | 2069 | G7M  | C2'-C3'-C4' | -2.81 | 96.89       | 102.64   |
| 2   | 2     | 1518 | MA6  | C1'-N9-C4   | -2.80 | 123.68      | 126.81   |
| 1   | 1     | 2457 | PSU  | C4'-O4'-C1' | -2.78 | 106.68      | 109.54   |
| 1   | 1     | 2503 | 2MA  | O4'-C1'-N9  | -2.75 | 102.91      | 108.11   |
| 1   | 1     | 2552 | OMU  | C5-C4-N3    | -2.75 | 116.53      | 123.28   |
| 1   | 1     | 955  | PSU  | C2'-C3'-C4' | -2.73 | 97.04       | 102.64   |
| 2   | 2     | 1207 | 2MG  | N3-C2-N1    | -2.70 | 122.15      | 126.19   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | 5     | 32   | 4OC  | O2'-C2'-C3' | -2.65 | 104.40      | 111.23   |
| 1   | 1     | 2504 | PSU  | C4'-O4'-C1' | -2.65 | 106.82      | 109.54   |
| 2   | 2     | 1402 | 4OC  | O4'-C4'-C3' | -2.54 | 100.00      | 105.16   |
| 1   | 1     | 2251 | OMG  | C2'-C1'-N9  | -2.54 | 106.22      | 113.48   |
| 1   | 1     | 1915 | 3TD  | C4'-O4'-C1' | -2.48 | 106.98      | 109.54   |
| 1   | 1     | 2504 | PSU  | C2'-C3'-C4' | -2.44 | 97.65       | 102.64   |
| 1   | 1     | 2457 | PSU  | C2'-C3'-C4' | -2.43 | 97.65       | 102.64   |
| 5   | 5     | 54   | 5MU  | C4'-O4'-C1' | -2.42 | 107.08      | 109.64   |
| 2   | 2     | 1518 | MA6  | C4'-O4'-C1' | -2.40 | 107.10      | 109.64   |
| 2   | 2     | 1519 | MA6  | C4'-O4'-C1' | -2.37 | 107.14      | 109.64   |
| 2   | 2     | 527  | 7MG  | C8-N9-C1'   | -2.35 | 115.38      | 122.43   |
| 1   | 1     | 2069 | G7M  | C1'-N9-C4   | -2.35 | 124.19      | 126.81   |
| 7   | 7     | 252  | MEQ  | OE1-CD-CG   | -2.29 | 118.00      | 121.97   |
| 1   | 1     | 1911 | PSU  | O2'-C2'-C1' | -2.25 | 107.02      | 111.93   |
| 1   | 1     | 2580 | PSU  | C4-C5-C1'   | -2.20 | 117.51      | 121.22   |
| 2   | 2     | 1516 | 2MG  | C1'-N9-C4   | -2.19 | 124.36      | 126.81   |
| 1   | 1     | 2445 | 2MG  | N3-C2-N1    | -2.19 | 122.92      | 126.19   |
| 1   | 1     | 1835 | 2MG  | N3-C2-N1    | -2.17 | 122.94      | 126.19   |
| 2   | 2     | 967  | 5MC  | C4'-O4'-C1' | -2.17 | 107.34      | 109.64   |
| 1   | 1     | 2504 | PSU  | C5-C6-N1    | -2.12 | 121.42      | 124.38   |
| 1   | 1     | 1618 | 6MZ  | C4'-O4'-C1' | -2.12 | 107.39      | 109.64   |
| 1   | 1     | 1915 | 3TD  | C5-C6-N1    | -2.12 | 121.42      | 124.38   |
| 1   | 1     | 2457 | PSU  | C5-C6-N1    | -2.12 | 121.43      | 124.38   |
| 1   | 1     | 2605 | PSU  | C5-C6-N1    | -2.10 | 121.45      | 124.38   |
| 49  | q     | 89   | 0TD  | O-C-CA      | -2.09 | 119.97      | 125.69   |
| 1   | 1     | 746  | PSU  | C5-C6-N1    | -2.09 | 121.47      | 124.38   |
| 2   | 2     | 1519 | MA6  | C2'-C3'-C4' | -2.09 | 98.36       | 102.64   |
| 1   | 1     | 955  | PSU  | C3'-C2'-C1' | -2.09 | 99.24       | 101.71   |
| 1   | 1     | 2580 | PSU  | C5-C6-N1    | -2.09 | 121.47      | 124.38   |
| 1   | 1     | 955  | PSU  | C5-C6-N1    | -2.08 | 121.48      | 124.38   |
| 2   | 2     | 1516 | 2MG  | N3-C2-N1    | -2.08 | 123.08      | 126.19   |
| 1   | 1     | 745  | 1MG  | C1'-N9-C4   | -2.08 | 124.49      | 126.81   |
| 2   | 2     | 516  | PSU  | C5-C6-N1    | -2.07 | 121.50      | 124.38   |
| 2   | 2     | 966  | 2MG  | N3-C2-N1    | -2.07 | 123.09      | 126.19   |
| 5   | 5     | 55   | PSU  | C5-C6-N1    | -2.06 | 121.51      | 124.38   |
| 2   | 2     | 1207 | 2MG  | O4'-C1'-N9  | 2.01  | 111.90      | 108.11   |
| 2   | 2     | 1498 | UR3  | C4'-O4'-C1' | 2.01  | 111.78      | 109.64   |
| 5   | 5     | 8    | 4SU  | O4'-C1'-N1  | 2.04  | 111.97      | 108.10   |
| 1   | 1     | 1915 | 3TD  | C3'-C2'-C1' | 2.04  | 104.13      | 101.71   |
| 1   | 1     | 2498 | OMC  | O3'-C3'-C4' | 2.06  | 117.15      | 111.01   |
| 1   | 1     | 2504 | PSU  | O4'-C1'-C2' | 2.06  | 106.92      | 104.69   |
| 5   | 5     | 54   | 5MU  | C5M-C5-C6   | 2.11  | 122.90      | 118.63   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 2   | 2     | 1516 | 2MG  | N2-C2-N3    | 2.11 | 119.39      | 116.94   |
| 1   | 1     | 747  | 5MU  | C5M-C5-C6   | 2.11 | 122.91      | 118.63   |
| 1   | 1     | 2504 | PSU  | C5-C1'-C2'  | 2.14 | 119.07      | 115.44   |
| 2   | 2     | 1402 | 4OC  | C4'-O4'-C1' | 2.14 | 111.92      | 109.64   |
| 1   | 1     | 747  | 5MU  | C2'-C1'-N1  | 2.17 | 119.30      | 113.46   |
| 2   | 2     | 516  | PSU  | O4'-C1'-C2' | 2.20 | 107.07      | 104.69   |
| 1   | 1     | 1618 | 6MZ  | C2'-C1'-N9  | 2.21 | 119.38      | 113.47   |
| 2   | 2     | 527  | 7MG  | C2-N3-C4    | 2.24 | 120.88      | 114.50   |
| 1   | 1     | 2445 | 2MG  | N2-C2-N3    | 2.27 | 119.57      | 116.94   |
| 1   | 1     | 2605 | PSU  | O4'-C1'-C2' | 2.28 | 107.16      | 104.69   |
| 2   | 2     | 1207 | 2MG  | N2-C2-N1    | 2.29 | 119.59      | 116.94   |
| 1   | 1     | 955  | PSU  | C5-C1'-C2'  | 2.33 | 119.39      | 115.44   |
| 1   | 1     | 2069 | G7M  | O4'-C1'-N9  | 2.39 | 112.63      | 108.11   |
| 1   | 1     | 1915 | 3TD  | O4'-C1'-C2' | 2.41 | 107.29      | 104.69   |
| 5   | 5     | 54   | 5MU  | C2'-C1'-N1  | 2.46 | 120.06      | 113.46   |
| 2   | 2     | 966  | 2MG  | N2-C2-N3    | 2.51 | 119.86      | 116.94   |
| 1   | 1     | 2445 | 2MG  | O3'-C3'-C4' | 2.55 | 118.62      | 111.01   |
| 1   | 1     | 2580 | PSU  | C3'-C2'-C1' | 2.57 | 104.76      | 101.71   |
| 1   | 1     | 2251 | OMG  | C4'-O4'-C1' | 2.60 | 112.40      | 109.64   |
| 5   | 5     | 32   | 4OC  | O3'-C3'-C4' | 2.71 | 119.10      | 111.01   |
| 1   | 1     | 1911 | PSU  | C3'-C2'-C1' | 2.73 | 104.95      | 101.71   |
| 1   | 1     | 1835 | 2MG  | N2-C2-N3    | 2.78 | 120.17      | 116.94   |
| 7   | 7     | 252  | MEQ  | CG-CD-NE2   | 2.92 | 121.04      | 116.49   |
| 1   | 1     | 746  | PSU  | O2'-C2'-C1' | 2.95 | 118.34      | 111.93   |
| 49  | q     | 89   | 0TD  | C-CA-N      | 2.97 | 116.50      | 109.95   |
| 2   | 2     | 966  | 2MG  | O3'-C3'-C2' | 2.98 | 121.47      | 111.86   |
| 1   | 1     | 745  | 1MG  | O2'-C2'-C3' | 3.02 | 121.63      | 111.86   |
| 1   | 1     | 2498 | OMC  | C6-C5-C4    | 3.06 | 118.64      | 117.44   |
| 1   | 1     | 1917 | PSU  | C3'-C2'-C1' | 3.07 | 105.35      | 101.71   |
| 1   | 1     | 1911 | PSU  | C4'-O4'-C1' | 3.14 | 112.78      | 109.54   |
| 5   | 5     | 32   | 4OC  | C6-C5-C4    | 3.17 | 118.66      | 117.42   |
| 5   | 5     | 20   | H2U  | O2'-C2'-C1' | 3.24 | 121.23      | 109.98   |
| 1   | 1     | 1962 | 5MC  | O3'-C3'-C4' | 3.24 | 120.69      | 111.01   |
| 1   | 1     | 2605 | PSU  | C5-C1'-C2'  | 3.26 | 120.97      | 115.44   |
| 1   | 1     | 2030 | 6MZ  | O3'-C3'-C2' | 3.33 | 122.63      | 111.86   |
| 1   | 1     | 2503 | 2MA  | O2'-C2'-C3' | 3.38 | 122.78      | 111.86   |
| 1   | 1     | 745  | 1MG  | O3'-C3'-C4' | 3.38 | 121.11      | 111.01   |
| 2   | 2     | 1519 | MA6  | C2-N1-C6    | 3.42 | 119.72      | 111.64   |
| 1   | 1     | 2457 | PSU  | C5-C1'-C2'  | 3.43 | 121.26      | 115.44   |
| 2   | 2     | 516  | PSU  | O2'-C2'-C1' | 3.56 | 119.66      | 111.93   |
| 1   | 1     | 1835 | 2MG  | O3'-C3'-C4' | 3.56 | 121.66      | 111.01   |
| 1   | 1     | 2030 | 6MZ  | O3'-C3'-C4' | 3.60 | 121.77      | 111.01   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 2   | 2     | 1516 | 2MG  | O3'-C3'-C2' | 3.65 | 123.67      | 111.86   |
| 2   | 2     | 1516 | 2MG  | O3'-C3'-C4' | 3.68 | 122.00      | 111.01   |
| 1   | 1     | 1835 | 2MG  | O3'-C3'-C2' | 3.69 | 123.80      | 111.86   |
| 5   | 5     | 32   | 4OC  | C2-N3-C4    | 3.72 | 120.16      | 115.43   |
| 2   | 2     | 1518 | MA6  | C2-N1-C6    | 3.74 | 120.47      | 111.64   |
| 1   | 1     | 2504 | PSU  | O2'-C2'-C1' | 3.81 | 120.20      | 111.93   |
| 1   | 1     | 2030 | 6MZ  | C2-N1-C6    | 3.82 | 119.22      | 116.47   |
| 1   | 1     | 1618 | 6MZ  | C2-N1-C6    | 3.88 | 119.26      | 116.47   |
| 1   | 1     | 2457 | PSU  | O2'-C2'-C1' | 3.91 | 120.42      | 111.93   |
| 2   | 2     | 1402 | 4OC  | C2-N3-C4    | 4.00 | 120.52      | 115.43   |
| 5   | 5     | 20   | H2U  | O3'-C3'-C4' | 4.03 | 123.06      | 111.01   |
| 5   | 5     | 55   | PSU  | O2'-C2'-C1' | 4.04 | 120.71      | 111.93   |
| 1   | 1     | 2580 | PSU  | O2'-C2'-C1' | 4.06 | 120.76      | 111.93   |
| 5   | 5     | 55   | PSU  | C5-C1'-C2'  | 4.14 | 122.46      | 115.44   |
| 1   | 1     | 2445 | 2MG  | O3'-C3'-C2' | 4.19 | 125.41      | 111.86   |
| 5   | 5     | 20   | H2U  | O3'-C3'-C2' | 4.29 | 125.71      | 111.86   |
| 1   | 1     | 955  | PSU  | O2'-C2'-C1' | 4.34 | 121.37      | 111.93   |
| 1   | 1     | 2605 | PSU  | O2'-C2'-C1' | 4.36 | 121.41      | 111.93   |
| 1   | 1     | 746  | PSU  | C5-C1'-C2'  | 4.43 | 122.95      | 115.44   |
| 1   | 1     | 746  | PSU  | O2'-C2'-C3' | 4.55 | 126.56      | 111.86   |
| 5   | 5     | 32   | 4OC  | O3'-C3'-C2' | 4.61 | 124.43      | 111.13   |
| 1   | 1     | 2605 | PSU  | O2'-C2'-C3' | 4.65 | 126.88      | 111.86   |
| 1   | 1     | 2503 | 2MA  | O3'-C3'-C4' | 4.68 | 124.98      | 111.01   |
| 2   | 2     | 1402 | 4OC  | C6-C5-C4    | 4.70 | 119.27      | 117.42   |
| 1   | 1     | 2580 | PSU  | O2'-C2'-C3' | 4.70 | 127.04      | 111.86   |
| 5   | 5     | 20   | H2U  | O2'-C2'-C3' | 4.73 | 127.13      | 111.86   |
| 1   | 1     | 2069 | G7M  | C2'-C1'-N9  | 4.75 | 126.17      | 113.47   |
| 1   | 1     | 745  | 1MG  | O3'-C3'-C2' | 4.77 | 127.28      | 111.86   |
| 1   | 1     | 2503 | 2MA  | O3'-C3'-C2' | 4.80 | 127.36      | 111.86   |
| 1   | 1     | 2457 | PSU  | O2'-C2'-C3' | 4.88 | 127.64      | 111.86   |
| 1   | 1     | 1618 | 6MZ  | O3'-C3'-C4' | 4.90 | 125.66      | 111.01   |
| 1   | 1     | 2069 | G7M  | O2'-C2'-C3' | 4.95 | 127.85      | 111.86   |
| 1   | 1     | 2503 | 2MA  | O2'-C2'-C1' | 4.95 | 127.12      | 111.61   |
| 1   | 1     | 2504 | PSU  | O2'-C2'-C3' | 5.00 | 128.01      | 111.86   |
| 1   | 1     | 955  | PSU  | O2'-C2'-C3' | 5.01 | 128.06      | 111.86   |
| 2   | 2     | 527  | 7MG  | C6-N1-C2    | 5.12 | 121.88      | 115.88   |
| 5   | 5     | 55   | PSU  | O2'-C2'-C3' | 5.12 | 128.40      | 111.86   |
| 2   | 2     | 1207 | 2MG  | C6-N1-C2    | 5.15 | 122.62      | 115.24   |
| 2   | 2     | 516  | PSU  | C5-C1'-C2'  | 5.16 | 124.20      | 115.44   |
| 1   | 1     | 2251 | OMG  | C6-N1-C2    | 5.21 | 121.98      | 115.88   |
| 2   | 2     | 967  | 5MC  | O3'-C3'-C2' | 5.28 | 128.91      | 111.86   |
| 2   | 2     | 1207 | 2MG  | C2-N3-C4    | 5.33 | 120.84      | 114.99   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1     | 2069 | G7M  | C6-N1-C2    | 5.41  | 122.22      | 115.88   |
| 2   | 2     | 516  | PSU  | O2'-C2'-C3' | 5.47  | 129.52      | 111.86   |
| 1   | 1     | 2580 | PSU  | C5-C1'-C2'  | 5.51  | 124.80      | 115.44   |
| 1   | 1     | 2069 | G7M  | O2'-C2'-C1' | 5.52  | 128.88      | 111.61   |
| 1   | 1     | 1939 | 5MU  | C4-N3-C2    | 5.60  | 119.83      | 115.16   |
| 2   | 2     | 966  | 2MG  | O3'-C3'-C4' | 5.88  | 128.58      | 111.01   |
| 1   | 1     | 2498 | OMC  | O3'-C3'-C2' | 5.92  | 128.22      | 111.13   |
| 1   | 1     | 1917 | PSU  | C4-N3-C2    | 6.08  | 120.23      | 115.16   |
| 1   | 1     | 1911 | PSU  | C4-N3-C2    | 6.12  | 120.26      | 115.16   |
| 2   | 2     | 966  | 2MG  | C6-N1-C2    | 6.20  | 124.11      | 115.24   |
| 2   | 2     | 1516 | 2MG  | C6-N1-C2    | 6.21  | 124.13      | 115.24   |
| 1   | 1     | 2445 | 2MG  | C6-N1-C2    | 6.26  | 124.20      | 115.24   |
| 1   | 1     | 1835 | 2MG  | C6-N1-C2    | 6.43  | 124.44      | 115.24   |
| 49  | q     | 89   | 0TD  | CSB-SB-CB   | 6.52  | 113.63      | 101.44   |
| 1   | 1     | 746  | PSU  | C3'-C2'-C1' | 7.71  | 110.86      | 101.71   |
| 2   | 2     | 527  | 7MG  | N3-C4-N9    | 9.22  | 138.91      | 126.98   |
| 1   | 1     | 2552 | OMU  | C4-N3-C2    | 9.50  | 124.22      | 114.21   |
| 1   | 1     | 747  | 5MU  | C4-N3-C2    | 11.35 | 124.63      | 115.16   |
| 1   | 1     | 746  | PSU  | C4-N3-C2    | 11.44 | 124.70      | 115.16   |
| 5   | 5     | 54   | 5MU  | C4-N3-C2    | 11.52 | 124.77      | 115.16   |
| 5   | 5     | 55   | PSU  | C4-N3-C2    | 11.57 | 124.81      | 115.16   |
| 1   | 1     | 2605 | PSU  | C4-N3-C2    | 11.60 | 124.83      | 115.16   |
| 1   | 1     | 2457 | PSU  | C4-N3-C2    | 11.66 | 124.89      | 115.16   |
| 1   | 1     | 955  | PSU  | C4-N3-C2    | 11.68 | 124.90      | 115.16   |
| 2   | 2     | 516  | PSU  | C4-N3-C2    | 11.69 | 124.91      | 115.16   |
| 1   | 1     | 2504 | PSU  | C4-N3-C2    | 11.74 | 124.96      | 115.16   |
| 1   | 1     | 2580 | PSU  | C4-N3-C2    | 11.81 | 125.01      | 115.16   |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 7   | 7     | 252 | MEQ  | CG-CD-NE2-CE |

There are no ring outliers.

15 monomers are involved in 26 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 1     | 1915 | 3TD  | 4       | 0            |
| 1   | 1     | 1917 | PSU  | 2       | 0            |
| 1   | 1     | 1939 | 5MU  | 3       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 1     | 2030 | 6MZ  | 2       | 0            |
| 1   | 1     | 2251 | OMG  | 3       | 0            |
| 1   | 1     | 2503 | 2MA  | 1       | 0            |
| 1   | 1     | 745  | 1MG  | 1       | 0            |
| 2   | 2     | 1402 | 4OC  | 1       | 0            |
| 2   | 2     | 1407 | 5MC  | 1       | 0            |
| 2   | 2     | 1518 | MA6  | 2       | 0            |
| 2   | 2     | 1519 | MA6  | 2       | 0            |
| 2   | 2     | 516  | PSU  | 1       | 0            |
| 2   | 2     | 966  | 2MG  | 4       | 0            |
| 2   | 2     | 967  | 5MC  | 1       | 0            |
| 5   | 5     | 20   | H2U  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 443 ligands modelled in this entry, 442 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 60  | FME  | 5     | 103 | 5    | 8,9,10       | 0.48 | 0           | 5,9,11      | 1.45 | 1 (20%)     |

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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 60  | FME  | 5     | 103 | 5    | -       | 0/6/9/11 | 0/0/0/0 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 60  | 5     | 103 | FME  | O-C-CA | -3.21 | 116.91                 | 125.69              |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.