



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

Feb 13, 2019 – 02:47 PM EST

PDB ID : 6GXN  
EMDB ID: : EMD-0081  
Title : Cryo-EM structure of an E. coli 70S ribosome in complex with RF3-GDPCP, RF1(GAQ) and Pint-tRNA (State III)  
Authors : Graf, M.; Huter, P.; Maracci, C.; Peterek, M.; Rodnina, M.V.; Wilson, D.N.  
Deposited on : 2018-06-27  
Resolution : 3.90 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

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

with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

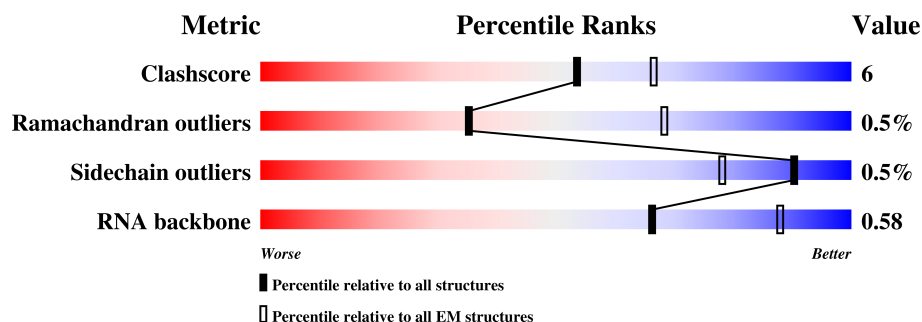
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 Å.

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
















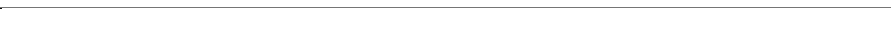

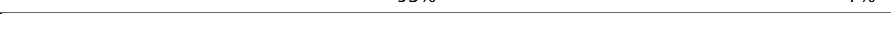
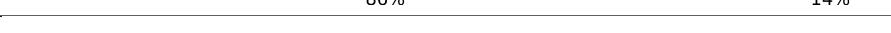
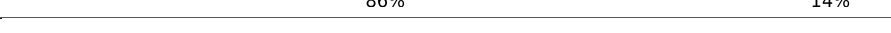







| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 136327                      | 1886                        |
| Ramachandran outliers | 132723                      | 1663                        |
| Sidechain outliers    | 132532                      | 1531                        |
| RNA backbone          | 3747                        | 458                         |

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   | A     | 2903   |                  |
| 2   | B     | 120    |                  |
| 3   | C     | 271    |                  |
| 4   | D     | 209    |                  |
| 5   | E     | 201    |                  |
| 6   | F     | 177    |                  |
| 7   | G     | 176    |                  |
| 8   | H     | 149    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 9   | I     | 141    |    |
| 10  | J     | 142    |    |
| 11  | K     | 122    |    |
| 12  | L     | 143    |    |
| 13  | M     | 136    |    |
| 14  | N     | 120    |    |
| 15  | O     | 116    |    |
| 16  | P     | 114    |    |
| 17  | Q     | 117    |    |
| 18  | R     | 103    |    |
| 19  | S     | 110    |    |
| 20  | T     | 93     |    |
| 21  | U     | 102    |  |
| 22  | V     | 94     |  |
| 23  | W     | 75     |  |
| 24  | X     | 77     |  |
| 25  | Y     | 63     |  |
| 26  | Z     | 58     |  |
| 27  | 0     | 56     |  |
| 28  | 1     | 50     |  |
| 29  | 2     | 46     |  |
| 30  | 3     | 64     |  |
| 31  | 4     | 38     |  |
| 32  | 5     | 131    |  |
| 33  | 7     | 7      |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 34  | a     | 1539   | 84% 15% .        |
| 35  | b     | 218    | 97% .            |
| 36  | c     | 206    | 99% .            |
| 37  | d     | 205    | 98% .            |
| 38  | e     | 157    | 97% ..           |
| 39  | f     | 100    | 97% ..           |
| 40  | g     | 151    | 99% .            |
| 41  | h     | 129    | 100%             |
| 42  | i     | 127    | 98% ..           |
| 43  | j     | 98     | 99% .            |
| 44  | k     | 116    | 99% .            |
| 45  | l     | 123    | 98% .            |
| 46  | m     | 114    | 98% .            |
| 47  | n     | 101    | 100%             |
| 48  | o     | 88     | 100%             |
| 49  | p     | 82     | 100%             |
| 50  | q     | 80     | 96% .            |
| 51  | r     | 65     | 100%             |
| 52  | s     | 79     | 100%             |
| 53  | t     | 85     | 100%             |
| 54  | u     | 65     | 98% .            |
| 55  | v     | 350    | 98% ..           |
| 56  | w     | 529    | 91% . 6%         |
| 57  | x     | 77     | 68% 30% .        |
| 58  | z     | 14     | 93% 7%           |

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 151860 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   | A     | 2895     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62153 | 27726 | 11439 | 20093 | 2895 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference     |
|-------|---------|----------|--------|----------|---------------|
| A     | 747     | C        | U      | conflict | GB 1036415628 |
| A     | 1847    | G        | A      | conflict | GB 1036415628 |

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 2   | B     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2572  | 1145 | 471 | 836 | 120 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference     |
|-------|---------|----------|--------|----------------|---------------|
| B     | 120     | A        | -      | expression tag | GB 1373146531 |

- Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | C     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | I     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | J     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 938   | 587 | 180 | 165 | 6 |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | L     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | M     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | N     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 15  | O     | 116      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | P     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 17  | Q     | 117      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | R     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | S     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | T     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 21  | U     | 102      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |  |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | V     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | W     | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 575   | 356 | 116 | 102 | 1 |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | X     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 25  | Y     | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L30.



| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | Z     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 27  | 0     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | 1     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 409   | 263 | 75 | 71 |   |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29  | 2     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 30  | 3     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31  | 4     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | 5     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 988   | 625 | 175 | 183 | 5 |         |       |

- Molecule 33 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 33  | 7     | 7        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 151   | 68 | 29 | 47 | 7 |         |       |

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 34  | a     | 1539     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33016 | 14725 | 6052 | 10700 | 1539 |         |       |

- Molecule 35 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | b     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1704  | 1081 | 305 | 311 | 7 |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36  | c     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 37  | d     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 38 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | e     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1141  | 709 | 218 | 208 | 6 |         |       |

- Molecule 39 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | f     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 817   | 515 | 148 | 148 | 6 |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | g     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1181  | 735 | 227 | 215 | 4 |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | h     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | i     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | j     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | k     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 869   | 535 | 173 | 158 | 3 |         |       |

- Molecule 45 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | l     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

- Molecule 46 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | m     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 883   | 546 | 178 | 156 | 3 |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | n     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 799   | 498 | 165 | 133 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| n     | 35      | ALA      | -      | insertion | UNP P0AG59 |

- Molecule 48 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | o     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 49 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | p     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 50 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | q     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |       |

- Molecule 51 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 51  | r     | 65       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 504   | 317 | 96 | 91 |         |       |

- Molecule 52 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | s     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 637   | 408 | 120 | 107 | 2 |         |       |

- Molecule 53 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | t     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |       |

- Molecule 54 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 54  | u     | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 495   | 307 | 100 | 87 | 1 |         |       |

- Molecule 55 is a protein called Peptide chain release factor RF1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 55  | v     | 348      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2436  | 1483 | 469 | 475 | 9 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| v     | 167     | CYS      | SER    | conflict | UNP P0A7I0 |

- Molecule 56 is a protein called Peptide chain release factor RF3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 56  | w     | 496      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3923  | 2487 | 674 | 742 | 20 |         |       |

- Molecule 57 is a RNA chain called fMet-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 57  | x     | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |       |

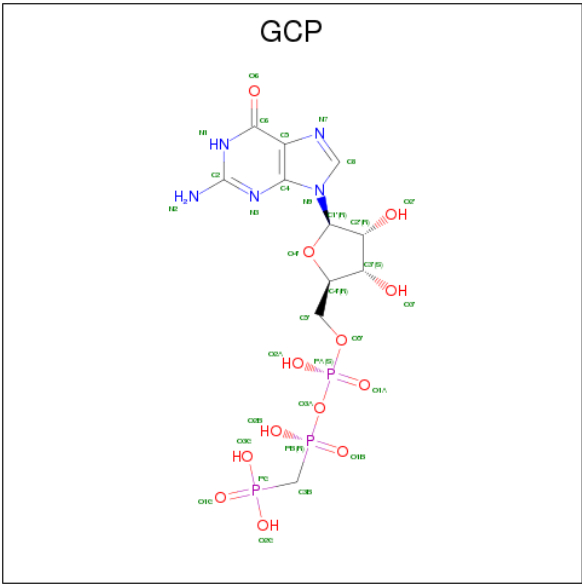
- Molecule 58 is a protein called Apidaecin.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 58  | z     | 14       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 120   | 80 | 25 | 15 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| z     | 10      | ARG      | GLN    | conflict | UNP Q8WSY8 |

- Molecule 59 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

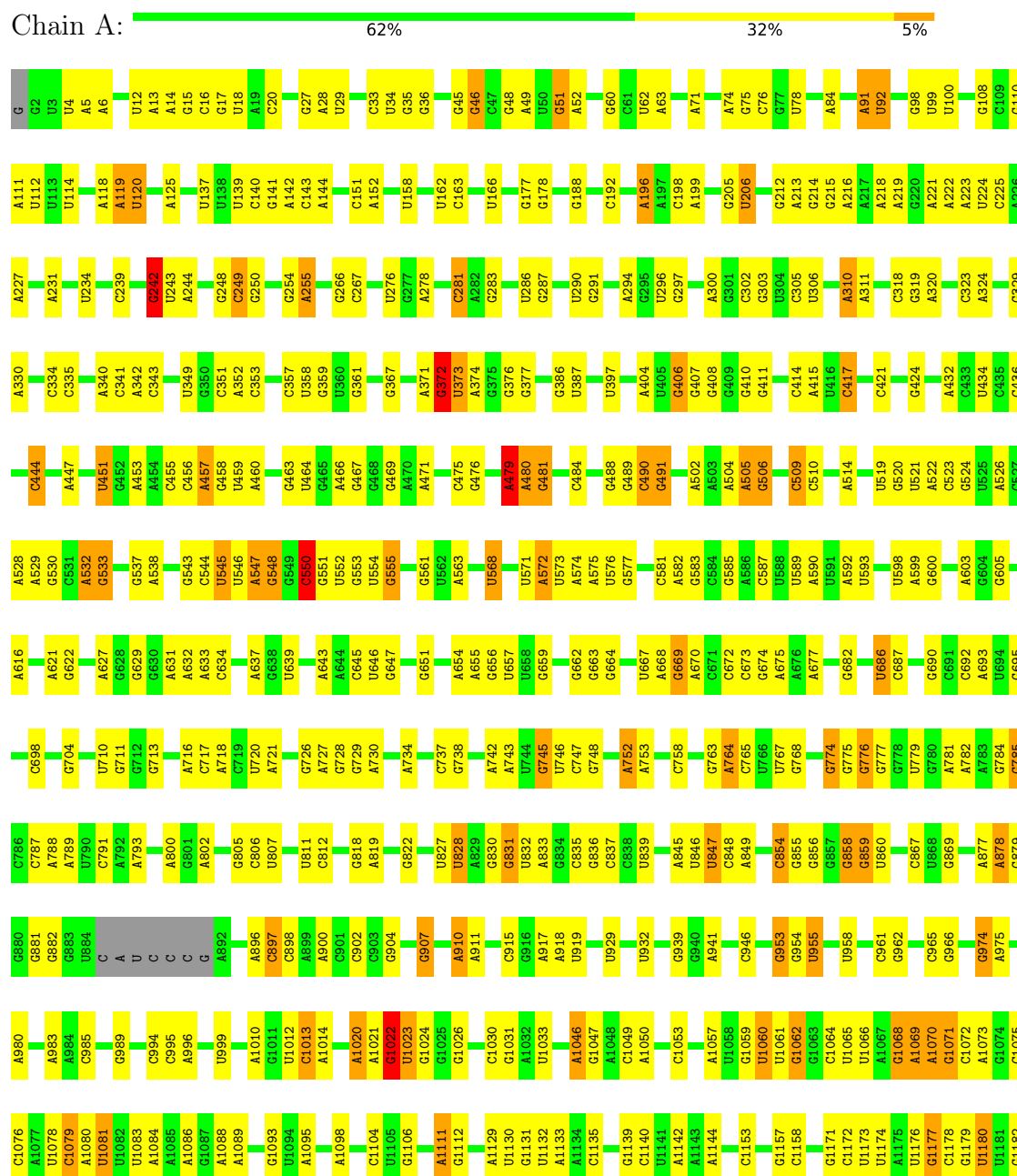


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
|     |       |          | Total | C  | N | O  | P |         |
| 59  | w     | 1        | 32    | 11 | 5 | 13 | 3 | 0       |

### 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 the various outlier classes 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.

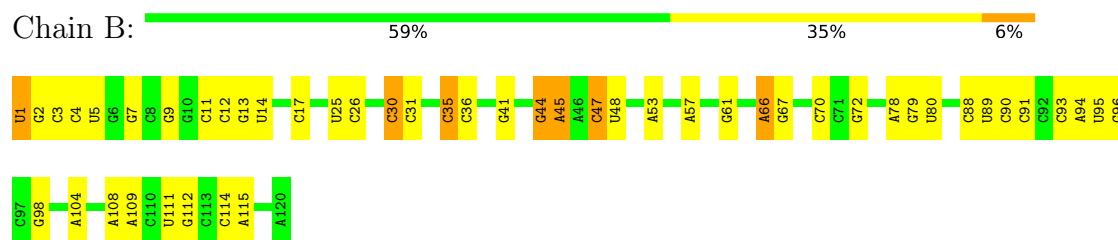
#### • Molecule 1: 23S ribosomal RNA



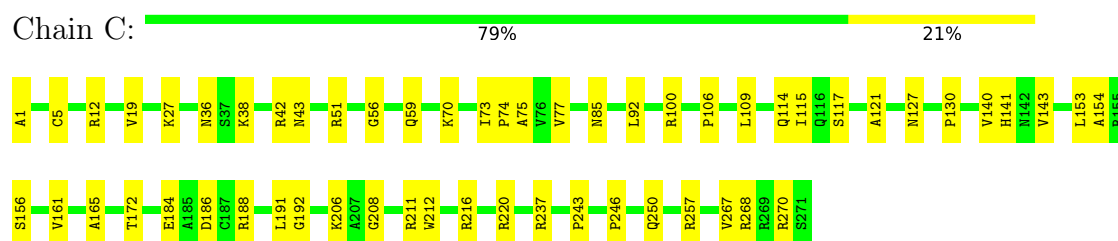
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| A2835 | U2743 | G2633 | G2523 | A2426 | A2322 | U2229 | G2112 | A2020 | U1911 | A1801 | G1682 | C1536 | C1399 | G1300 | U1188 |
| U2836 | G2744 | A2634 | G2529 | G2427 | G2325 | G2230 | U2113 | C2021 | A1912 | A1802 | G1687 | G1537 | G1416 | A1301 | A1189 |
| A2837 | G2745 | A2635 | A2530 | G2428 | C2326 | G2233 | U2118 | U2022 | A1913 | C1806 | G1687 | A1544 | C1417 | C1306 | G1190 |
| G2847 | G2746 | C2636 | A2531 | G2429 | A2327 | G2234 | A2119 | G2024 | A1915 | G1807 | C1694 | G1555 | A1418 | G1309 | G1202 |
| G2848 | G2747 | C2646 | G2535 | A2430 | A2328 | G2235 | G2120 | U2028 | A1916 | A1808 | G1695 | G1559 | A1419 | G1203 | U1203 |
| U2849 | A2748 | U2647 | G2536 | A2435 | U2329 | G2238 | G2127 | U2029 | U1917 | A1810 | G1699 | U1559 | G1420 | A1204 | A1204 |
|       |       | G2648 | G2539 | U2441 | G2330 | G2239 | U2131 | A2030 | G1921 | G1811 | A1700 | U1560 | G1421 | A1205 | G1206 |
| U2861 | C2752 | G2654 | A2547 | C2442 | A2333 | U2240 | U2132 | A2031 | G1922 | U1812 | A1701 | C1565 | C1422 | C1314 | G1206 |
| G2862 | G2753 | A2655 | U2552 | G2443 | A2334 | G2241 | G2133 | U2034 | A1928 | G1816 | G1704 | C1569 | C1428 | U1313 | U1209 |
| G2863 | C2755 | U2656 | G2555 | U2444 | A2335 | G2242 | G2136 | G2035 | A1929 | G1817 | A1705 | A1569 | G1430 | A1321 | U1210 |
| G2864 | C2762 | G2659 | U2554 | G2447 | A2336 | U2243 | G2140 | U2037 | G1930 | U1818 | G1715 | U1578 | A1431 | A1322 | C1211 |
|       | G2763 | U2662 | C2559 | A2448 | C2342 | G2244 | G2141 | A2037 | A1936 | G1823 | G1716 | A1579 | G1432 | G1323 | G1212 |
| U2872 | A2765 | A2665 | C2560 | A2450 | G2345 | U2247 | G2144 | G2043 | A1937 | U1827 | G1724 | C1585 | G1435 | G1215 | G1215 |
| A2873 | U2768 | C2666 | A2564 | C2456 | G2347 | G2248 | G2145 | C2047 | A1938 | G1828 | G1729 | C1592 | G1436 | U1329 | U1222 |
|       | U2769 | G2673 | A2565 | U2457 | U2348 | G2250 | C2146 | G2048 | U1940 | A1829 | U1729 | A1593 | C1447 | U1330 | U1223 |
| C2880 | C2770 | U2676 | A2566 | G2458 | G2349 | G2251 | A2147 | G2049 | C1941 | G1831 | G1730 | A1597 | C1447 | U1331 | U1224 |
| U2884 | C2771 | C2676 | G2567 | A2459 | C2350 | C2254 | G2157 | C2050 | U1944 | C1832 | G1731 | A1598 | C1450 | G1332 | G1225 |
|       | A2776 |       |       | U2460 | C2354 | C2258 | G2162 | A2051 | U1945 | U1833 | G1732 | A1598 | C1451 | G1333 | A1226 |
| A2893 | G2777 | G2682 | G2570 | A2468 | G2357 | C2268 | C2163 | A2052 | G1965 | U1835 | G1733 | A1603 | G1452 | G1334 | G1227 |
| G2894 | U2778 | C2683 | U2571 |       |       | A2268 | A2164 | C2055 | A1953 | G1839 | G1737 | C1607 | C1453 | G1341 | A1237 |
| U2898 | G2779 | A2687 | A2572 | U2473 | G2360 | G2271 | C2165 | G2056 | G1954 | G1840 | G1738 | C1607 | C1454 | U1242 | U1242 |
| A2899 | A2781 | G2688 | C2573 | G2474 | G2361 | G2271 | A2170 | A2060 | U1955 | U1841 | A1744 | A1610 | C1461 | C1345 | U1243 |
| A2900 | C2782 | U2689 | U2580 | A2476 | G2370 | G2279 | A2171 | A2061 | U1956 | G1842 | A1745 | C1611 | C1469 | C1348 | A1244 |
| C2901 | G2788 | G2690 | G2581 |       | G2371 | C2283 | U2172 | A2062 | A1960 |       | A1746 | C1612 |       | C1349 |       |
| C2902 |       | C2691 | G2582 | C2483 | G2372 | G2286 | A2173 | A2063 | G1961 | G1847 |       |       |       |       | A1247 |
|       | G2791 | G2692 | U2585 | G2484 | U2373 | A2287 | C2174 | U2068 | U1962 | A1848 | G1753 | A1634 | G1475 | A1353 | U1248 |
|       | C2794 | U2693 | U2586 | U2491 | C2374 | A2288 | C2175 | G2069 | U1963 |       | G1754 | A1635 | U1476 | A1354 | U1249 |
| U2808 | C2795 | U2698 | A2590 | G2494 | G2383 | A2289 | C2176 | A2070 | G1967 | A1858 | A1757 | U1636 | G1482 | G1355 | G1250 |
| G2809 | U2796 | C2703 | A2598 | G2495 | U2384 | G2289 | C2177 | A2071 | U1970 | G1862 | U1758 | A1637 | G1490 | G1356 | C1251 |
| U2797 | G2797 | C2704 | A2602 | C2496 | C2385 | G2290 | C2178 | C2072 | A1971 |       | U1759 | C1646 | A1490 | A1365 | G1252 |
| U2798 | U2798 | G2712 | G2603 | A2497 | G2386 | U2291 | C2179 | C2073 | U1972 | C1870 | G1760 | U1647 | G1491 | A1253 | A1253 |
| A2800 | A2800 | U2713 | U2604 | C2498 | A2391 | U2292 | C2185 | U2076 | G1972 | A1871 | C1764 | U1648 | G1492 | U1254 | U1255 |
| G2801 | G2801 | G2714 | U2605 | G2502 | U2393 | G2293 | G2186 | U2077 | G1986 | A1872 |       |       | C1493 | G1369 | G1256 |
| G2802 | C2715 | C2715 | U2609 | U2503 | C2394 | G2295 | U2189 | U2078 | U1986 | G1873 |       |       |       | U1372 |       |
|       | C2716 | C2716 | U2610 | U2504 | G2395 | U2296 | U2192 | A2081 | A1987 | U1880 | G1773 | G1651 | G1500 | G1376 | G1266 |
|       | U2808 | C2717 | U2611 | U2505 | G2396 | A2297 | U2192 | A2082 | U1991 |       | C1774 |       | A1504 | C1376 | A1269 |
|       | A2809 | G2718 | U2612 | U2506 | C2402 | C2300 | A2198 | U2086 | G1992 | G1884 | U1779 | G1660 | A1504 | G1377 | C1270 |
| U2818 | G2818 | G2719 | A2613 | C2507 | U2403 | G2305 | G2204 | U2087 | U1996 | G1892 | U1780 | G1661 | A1509 | A1378 | G1271 |
| A2820 | A2820 | U2720 | U2614 | G2508 | U2404 | G2306 | A2211 | G2094 | G1997 | C1893 | U1781 | G1662 | G1510 | A1272 | A1272 |
| G2822 | G2822 | C2721 | U2615 | C2509 | G2405 | G2307 | U2212 | C2096 | U1998 | G1896 | U1782 | G1663 | G1510 | G1380 |       |
| A2823 | A2823 | U2726 | G2618 | G2415 | G2416 | G2308 | U2213 | C2097 | G1999 | A1783 |       | A1664 | A1515 | A1383 | A1287 |
| C2824 | C2824 | C2417 | U2619 | C2517 | C2417 | G2309 | U2214 | G2100 | G2002 | A1784 |       | A1665 | U1522 | A1386 | G1289 |
| G2825 | G2825 | C2418 | U2620 | C2518 | C2418 | G2310 | U2215 | U2007 | U1999 | A1787 |       | A1666 | U1523 | C1386 | C1290 |
|       |       | U2731 | U2621 | C2519 | C2419 | G2311 | U2216 | G2101 | U2008 | U1796 | U1797 | C1670 | G1524 | A1387 | C1291 |
| U2832 | G2732 | G2732 | U2622 | A2518 | U2423 | G2312 | G2216 | A2108 | C2008 | G1797 |       | A1532 | A1532 | U1394 | G1293 |
| U2833 | A2733 | G2631 | G2630 | U2519 | C2424 | U2320 | A2225 | U2109 | A2009 | G1798 |       | U1533 | A1533 | A1395 | U1294 |
| G2834 | U2739 | A2632 | A2632 | U2520 | A2425 | U2321 | C2226 | G2111 | G1907 | G1907 | C1800 | C1675 | A1535 | C1398 | G1296 |



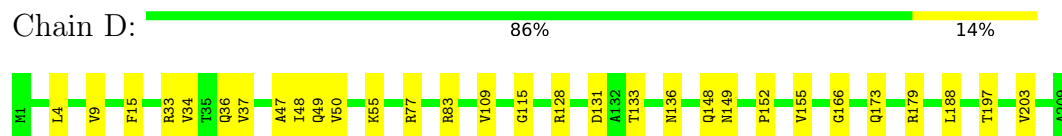
- Molecule 2: 5S ribosomal RNA



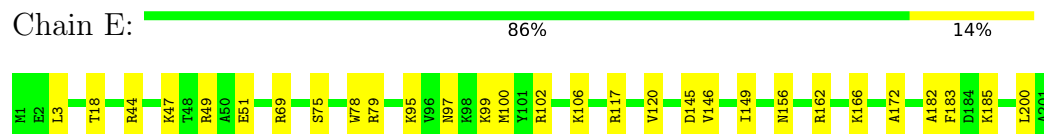
- Molecule 3: 50S ribosomal protein L2



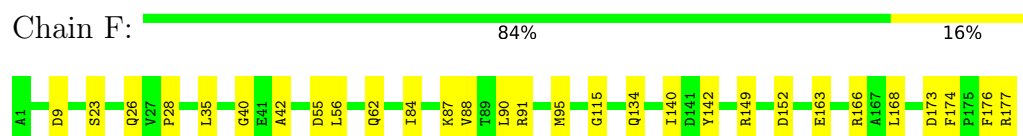
- Molecule 4: 50S ribosomal protein L3



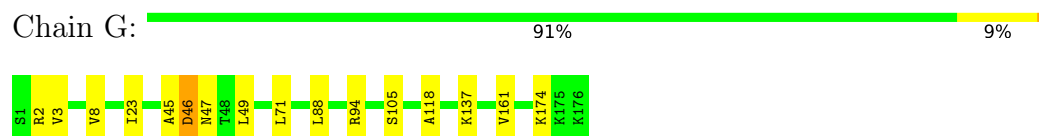
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9





- Molecule 9: 50S ribosomal protein L11

Chain I: 87% 13%



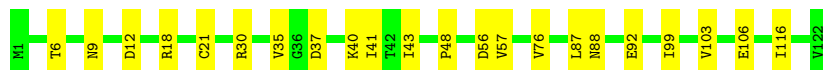
- Molecule 10: 50S ribosomal protein L13

Chain J: 87% 13%



- Molecule 11: 50S ribosomal protein L14

Chain K: 82% 18%



- Molecule 12: 50S ribosomal protein L15

Chain L: 87% 13%



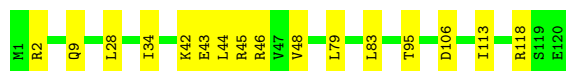
- Molecule 13: 50S ribosomal protein L16

Chain M: 85% 14%



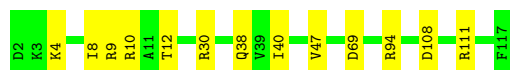
- Molecule 14: 50S ribosomal protein L17

Chain N: 87% 13%

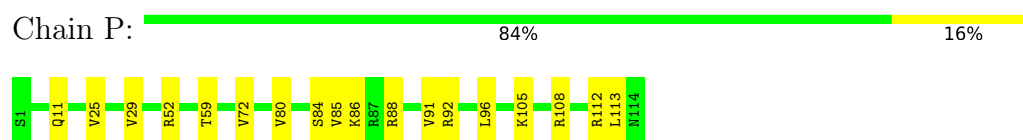


- Molecule 15: 50S ribosomal protein L18

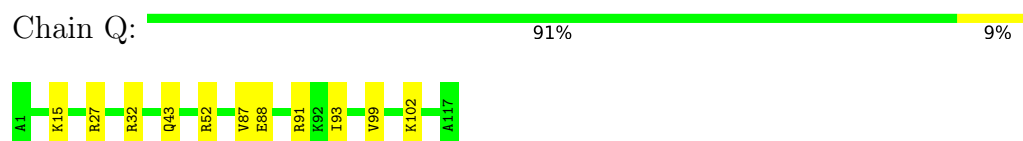
Chain O: 89% 11%



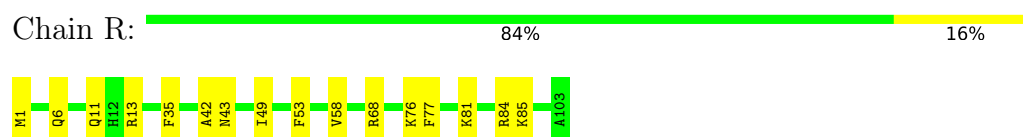
- Molecule 16: 50S ribosomal protein L19



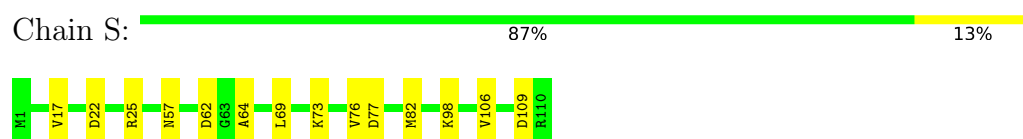
- Molecule 17: 50S ribosomal protein L20



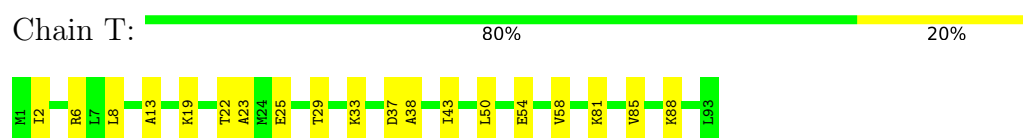
- Molecule 18: 50S ribosomal protein L21



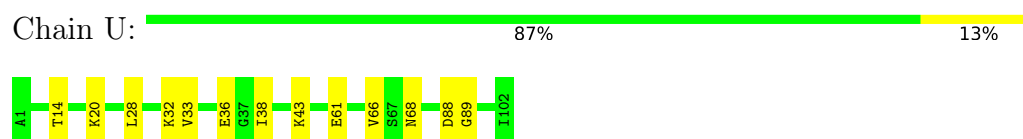
- Molecule 19: 50S ribosomal protein L22



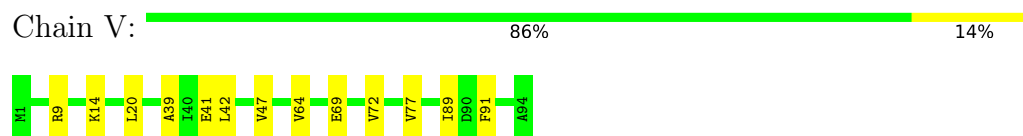
- Molecule 20: 50S ribosomal protein L23



- Molecule 21: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L25




- Molecule 23: 50S ribosomal protein L27

Chain W:  93% 7%



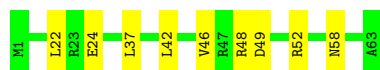
- Molecule 24: 50S ribosomal protein L28

Chain X:  86% 14%




- Molecule 25: 50S ribosomal protein L29

Chain Y:  86% 14%




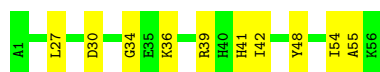
- Molecule 26: 50S ribosomal protein L30

Chain Z:  88% 12%




- Molecule 27: 50S ribosomal protein L32

Chain 0:  82% 18%



- Molecule 28: 50S ribosomal protein L33

Chain 1:  90% 10%



- Molecule 29: 50S ribosomal protein L34

Chain 2:  72% 28%



- Molecule 30: 50S ribosomal protein L35

Chain 3:  73% 25% .



- Molecule 31: 50S ribosomal protein L36

Chain 4: 82% 16% .



- Molecule 32: 50S ribosomal protein L10

Chain 5: 80% 20%



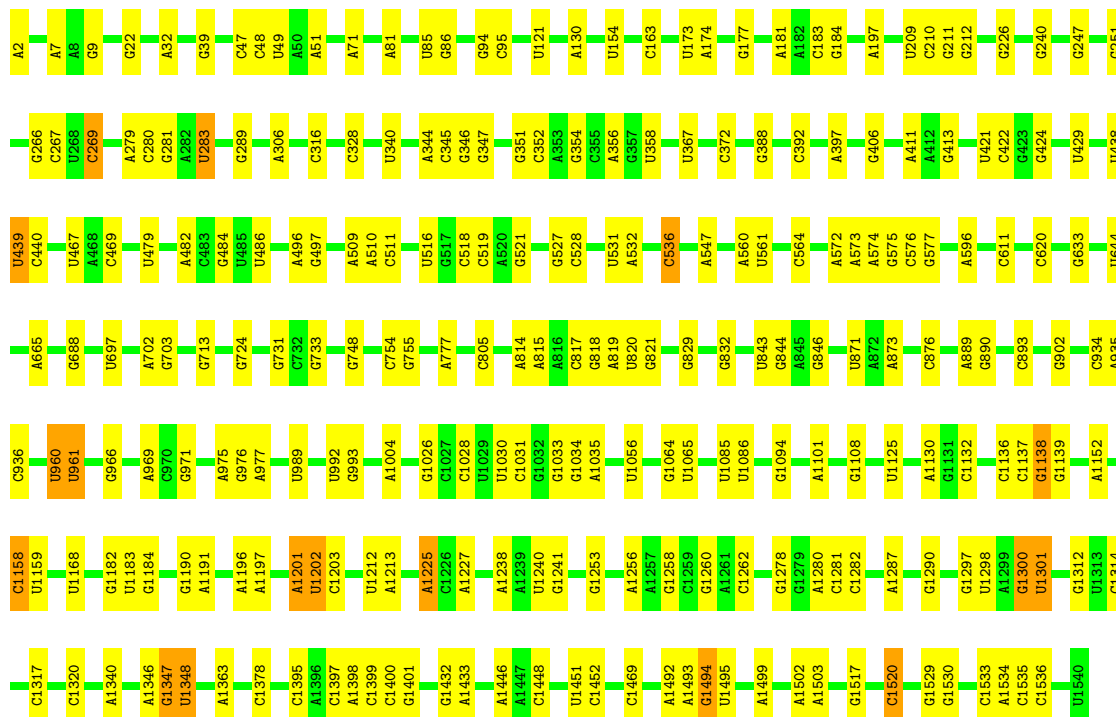
- Molecule 33: mRNA

Chain 7: 86% 14%



- Molecule 34: 16S ribosomal RNA

Chain a: 84% 15% .



- Molecule 35: 30S ribosomal protein S2

Chain b:  97% .



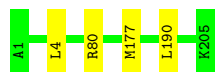
- Molecule 36: 30S ribosomal protein S3

Chain c:  99% .



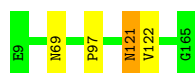
- Molecule 37: 30S ribosomal protein S4

Chain d:  98% .



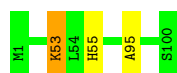
- Molecule 38: 30S ribosomal protein S5

Chain e:  97% ..



- Molecule 39: 30S ribosomal protein S6

Chain f:  97% ..



- Molecule 40: 30S ribosomal protein S7

Chain g:  99% .



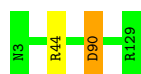
- Molecule 41: 30S ribosomal protein S8

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: 30S ribosomal protein S9

Chain i:  98% ..



- Molecule 43: 30S ribosomal protein S10

Chain j:  99%



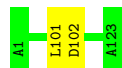
- Molecule 44: 30S ribosomal protein S11

Chain k:  99%



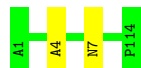
- Molecule 45: 30S ribosomal protein S12

Chain l:  98%



- Molecule 46: 30S ribosomal protein S13

Chain m:  98%



- Molecule 47: 30S ribosomal protein S14

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 30S ribosomal protein S15

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 30S ribosomal protein S16

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 50: 30S ribosomal protein S17

Chain q:  96%



- Molecule 51: 30S ribosomal protein S18

Chain r: 100%

There are no outlier residues recorded for this chain.

- Molecule 52: 30S ribosomal protein S19

Chain s: 100%

There are no outlier residues recorded for this chain.

- Molecule 53: 30S ribosomal protein S20

Chain t: 100%

There are no outlier residues recorded for this chain.

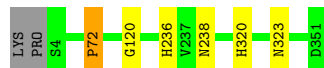
- Molecule 54: 30S ribosomal protein S21

Chain u: 98%



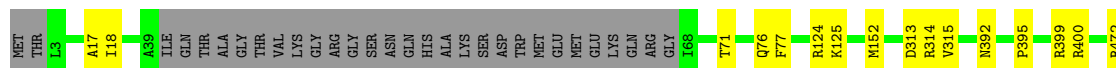
- Molecule 55: Peptide chain release factor RF1

Chain v: 98%



- Molecule 56: Peptide chain release factor RF3

Chain w: 91% 6%



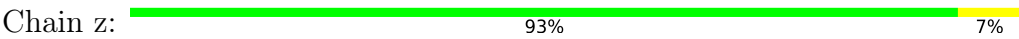
- Molecule 57: fMet-tRNA

Chain x: 68% 30%



- Molecule 58: Apidaecin





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 54142                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 45.9                                    | Depositor |
| Minimum defocus (nm)                 | Not provided                            | Depositor |
| Maximum defocus (nm)                 | Not provided                            | Depositor |
| Magnification                        | Not provided                            | Depositor |
| Image detector                       | FEI FALCON II (4k x 4k)                 | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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   | A     | 0.29         | 0/69612        | 1.00        | 222/108599 (0.2%) |
| 10  | J     | 0.25         | 0/1152         | 0.46        | 0/1551            |
| 11  | K     | 0.28         | 0/947          | 0.53        | 0/1268            |
| 12  | L     | 0.28         | 0/1054         | 0.54        | 0/1403            |
| 13  | M     | 0.27         | 0/1093         | 0.58        | 1/1460 (0.1%)     |
| 14  | N     | 0.27         | 0/973          | 0.52        | 0/1301            |
| 15  | O     | 0.25         | 0/902          | 0.47        | 0/1209            |
| 16  | P     | 0.25         | 0/929          | 0.52        | 1/1242 (0.1%)     |
| 17  | Q     | 0.26         | 0/960          | 0.45        | 0/1278            |
| 18  | R     | 0.26         | 0/829          | 0.51        | 0/1107            |
| 19  | S     | 0.24         | 0/864          | 0.50        | 0/1156            |
| 2   | B     | 0.39         | 1/2876 (0.0%)  | 1.16        | 32/4483 (0.7%)    |
| 20  | T     | 0.26         | 0/744          | 0.50        | 0/994             |
| 21  | U     | 0.29         | 0/787          | 0.56        | 0/1051            |
| 22  | V     | 0.25         | 0/766          | 0.48        | 0/1025            |
| 23  | W     | 0.26         | 0/582          | 0.42        | 0/769             |
| 24  | X     | 0.24         | 0/635          | 0.46        | 0/848             |
| 25  | Y     | 0.23         | 0/510          | 0.47        | 0/677             |
| 26  | Z     | 0.24         | 0/453          | 0.46        | 0/605             |
| 27  | 0     | 0.24         | 0/450          | 0.46        | 0/599             |
| 28  | 1     | 0.26         | 0/416          | 0.50        | 0/554             |
| 29  | 2     | 0.25         | 0/380          | 0.50        | 0/498             |
| 3   | C     | 0.26         | 0/2121         | 0.51        | 0/2852            |
| 30  | 3     | 0.25         | 0/513          | 0.64        | 1/676 (0.1%)      |
| 31  | 4     | 0.26         | 0/303          | 0.52        | 0/397             |
| 32  | 5     | 0.31         | 0/1001         | 0.63        | 0/1350            |
| 33  | 7     | 0.33         | 0/169          | 0.87        | 0/261             |
| 34  | a     | 0.29         | 1/36967 (0.0%) | 0.98        | 84/57666 (0.1%)   |
| 35  | b     | 0.28         | 0/1735         | 0.55        | 0/2338            |
| 36  | c     | 0.26         | 0/1651         | 0.48        | 0/2225            |
| 37  | d     | 0.27         | 0/1665         | 0.54        | 2/2227 (0.1%)     |
| 38  | e     | 0.28         | 0/1154         | 0.58        | 0/1554            |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >2         | RMSZ        | # Z  >2           |
| 39  | f     | 0.31         | 0/835           | 0.62        | 0/1128            |
| 4   | D     | 0.26         | 0/1586          | 0.51        | 0/2134            |
| 40  | g     | 0.27         | 0/1195          | 0.52        | 0/1602            |
| 41  | h     | 0.26         | 0/989           | 0.55        | 0/1326            |
| 42  | i     | 0.27         | 0/1034          | 0.56        | 0/1375            |
| 43  | j     | 0.27         | 0/796           | 0.60        | 0/1077            |
| 44  | k     | 0.27         | 0/885           | 0.51        | 0/1195            |
| 45  | l     | 0.28         | 0/969           | 0.59        | 0/1300            |
| 46  | m     | 0.26         | 0/892           | 0.55        | 0/1193            |
| 47  | n     | 0.24         | 0/811           | 0.50        | 0/1081            |
| 48  | o     | 0.24         | 0/722           | 0.53        | 0/964             |
| 49  | p     | 0.26         | 0/659           | 0.50        | 0/884             |
| 5   | E     | 0.25         | 0/1571          | 0.47        | 0/2113            |
| 50  | q     | 0.27         | 0/657           | 0.58        | 0/881             |
| 51  | r     | 0.24         | 0/511           | 0.48        | 0/689             |
| 52  | s     | 0.26         | 0/652           | 0.49        | 0/877             |
| 53  | t     | 0.29         | 0/671           | 0.49        | 0/888             |
| 54  | u     | 0.32         | 0/500           | 0.65        | 0/668             |
| 55  | v     | 0.27         | 0/2468          | 0.53        | 1/3351 (0.0%)     |
| 56  | w     | 0.29         | 0/3996          | 0.63        | 2/5402 (0.0%)     |
| 57  | x     | 0.32         | 0/1832          | 1.16        | 18/2855 (0.6%)    |
| 58  | z     | 0.25         | 0/127           | 0.50        | 0/175             |
| 6   | F     | 0.32         | 0/1434          | 0.55        | 0/1926            |
| 7   | G     | 0.26         | 0/1343          | 0.52        | 0/1816            |
| 8   | H     | 0.26         | 0/1122          | 0.47        | 0/1515            |
| 9   | I     | 0.29         | 0/1046          | 0.55        | 0/1410            |
| All | All   | 0.29         | 2/164496 (0.0%) | 0.89        | 364/245048 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 11  | K     | 0                   | 1                   |
| 13  | M     | 0                   | 1                   |
| 18  | R     | 0                   | 1                   |
| 21  | U     | 0                   | 1                   |
| 30  | 3     | 0                   | 2                   |
| 32  | 5     | 0                   | 1                   |
| 35  | b     | 0                   | 3                   |
| 38  | e     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 39  | f     | 0                   | 2                   |
| 42  | i     | 0                   | 1                   |
| 43  | j     | 0                   | 1                   |
| 45  | l     | 0                   | 1                   |
| 46  | m     | 0                   | 1                   |
| 50  | q     | 0                   | 1                   |
| 55  | v     | 0                   | 1                   |
| 56  | w     | 0                   | 3                   |
| 6   | F     | 0                   | 2                   |
| 7   | G     | 0                   | 3                   |
| All | All   | 0                   | 27                  |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 34  | a     | 2   | A    | OP3-P | -10.54 | 1.48        | 1.61     |
| 2   | B     | 1   | U    | OP3-P | -10.53 | 1.48        | 1.61     |

All (364) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 2604 | U    | C2-N1-C1' | 10.47 | 130.26      | 117.70   |
| 1   | A     | 2063 | C    | N1-C2-O2  | 9.84  | 124.80      | 118.90   |
| 1   | A     | 2506 | U    | C2-N1-C1' | 9.62  | 129.25      | 117.70   |
| 2   | B     | 36   | C    | N1-C2-O2  | 9.44  | 124.56      | 118.90   |
| 1   | A     | 2506 | U    | N1-C2-O2  | 9.31  | 129.31      | 122.80   |
| 1   | A     | 1313 | U    | N3-C2-O2  | -9.11 | 115.82      | 122.20   |
| 1   | A     | 2226 | C    | N1-C2-O2  | 9.07  | 124.34      | 118.90   |
| 1   | A     | 1348 | C    | N1-C2-O2  | 9.00  | 124.30      | 118.90   |
| 1   | A     | 1326 | U    | N3-C2-O2  | -8.96 | 115.93      | 122.20   |
| 1   | A     | 2473 | U    | N1-C2-O2  | 8.82  | 128.98      | 122.80   |
| 1   | A     | 2604 | U    | C6-N1-C1' | -8.73 | 108.98      | 121.20   |
| 1   | A     | 2506 | U    | N3-C2-O2  | -8.72 | 116.10      | 122.20   |
| 1   | A     | 2473 | U    | N3-C2-O2  | -8.61 | 116.17      | 122.20   |
| 56  | w     | 399  | ARG  | N-CA-C    | 8.51  | 133.99      | 111.00   |
| 34  | a     | 611  | C    | N1-C2-O2  | 8.47  | 123.98      | 118.90   |
| 1   | A     | 1313 | U    | N1-C2-O2  | 8.46  | 128.72      | 122.80   |
| 1   | A     | 1326 | U    | N1-C2-O2  | 8.44  | 128.71      | 122.80   |
| 1   | A     | 955  | U    | C2-N1-C1' | 8.28  | 127.63      | 117.70   |
| 1   | A     | 847  | U    | N3-C2-O2  | -8.27 | 116.41      | 122.20   |
| 1   | A     | 2794 | C    | N3-C2-O2  | -8.21 | 116.16      | 121.90   |
| 1   | A     | 2063 | C    | C2-N1-C1' | 8.20  | 127.81      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 1313 | U    | C2-N1-C1'  | 8.16  | 127.49      | 117.70   |
| 2   | B     | 36   | C    | N3-C2-O2   | -8.16 | 116.19      | 121.90   |
| 1   | A     | 2063 | C    | N3-C2-O2   | -8.12 | 116.21      | 121.90   |
| 2   | B     | 35   | C    | N1-C2-O2   | 8.03  | 123.72      | 118.90   |
| 1   | A     | 1774 | C    | N3-C2-O2   | -8.02 | 116.29      | 121.90   |
| 57  | x     | 67   | C    | N1-C2-O2   | 7.97  | 123.68      | 118.90   |
| 1   | A     | 847  | U    | N1-C2-O2   | 7.96  | 128.37      | 122.80   |
| 2   | B     | 26   | C    | N1-C2-O2   | 7.90  | 123.64      | 118.90   |
| 1   | A     | 2072 | C    | C2-N1-C1'  | 7.87  | 127.46      | 118.80   |
| 1   | A     | 2457 | U    | C2-N1-C1'  | 7.72  | 126.96      | 117.70   |
| 1   | A     | 1180 | U    | N1-C2-O2   | 7.68  | 128.18      | 122.80   |
| 1   | A     | 2473 | U    | C2-N1-C1'  | 7.62  | 126.84      | 117.70   |
| 1   | A     | 1893 | C    | N3-C2-O2   | -7.61 | 116.57      | 121.90   |
| 1   | A     | 1893 | C    | N1-C2-O2   | 7.61  | 123.47      | 118.90   |
| 2   | B     | 12   | C    | N1-C2-O2   | 7.59  | 123.46      | 118.90   |
| 1   | A     | 847  | U    | C2-N1-C1'  | 7.58  | 126.80      | 117.70   |
| 34  | a     | 754  | C    | C2-N1-C1'  | 7.56  | 127.12      | 118.80   |
| 1   | A     | 2580 | U    | C2-N1-C1'  | 7.50  | 126.70      | 117.70   |
| 34  | a     | 1348 | U    | N1-C2-O2   | 7.42  | 128.00      | 122.80   |
| 1   | A     | 2604 | U    | O4'-C1'-N1 | 7.41  | 114.13      | 108.20   |
| 57  | x     | 25   | U    | C2-N1-C1'  | 7.32  | 126.48      | 117.70   |
| 1   | A     | 2226 | C    | N3-C2-O2   | -7.25 | 116.82      | 121.90   |
| 1   | A     | 1326 | U    | C2-N1-C1'  | 7.24  | 126.39      | 117.70   |
| 1   | A     | 2063 | C    | C6-N1-C2   | -7.24 | 117.41      | 120.30   |
| 1   | A     | 1180 | U    | N3-C2-O2   | -7.17 | 117.18      | 122.20   |
| 2   | B     | 36   | C    | C2-N1-C1'  | 7.16  | 126.68      | 118.80   |
| 1   | A     | 867  | C    | N1-C2-O2   | 7.12  | 123.17      | 118.90   |
| 1   | A     | 1914 | C    | C6-N1-C2   | -7.12 | 117.45      | 120.30   |
| 1   | A     | 752  | A    | P-O3'-C3'  | 7.08  | 128.19      | 119.70   |
| 1   | A     | 1348 | C    | N3-C2-O2   | -7.07 | 116.95      | 121.90   |
| 1   | A     | 1378 | A    | P-O3'-C3'  | 7.03  | 128.13      | 119.70   |
| 1   | A     | 1774 | C    | N1-C2-O2   | 7.01  | 123.11      | 118.90   |
| 2   | B     | 36   | C    | C6-N1-C2   | -7.00 | 117.50      | 120.30   |
| 1   | A     | 2226 | C    | C2-N1-C1'  | 6.97  | 126.47      | 118.80   |
| 1   | A     | 2580 | U    | O4'-C1'-N1 | 6.89  | 113.72      | 108.20   |
| 1   | A     | 854  | C    | N3-C2-O2   | -6.88 | 117.08      | 121.90   |
| 34  | a     | 1158 | C    | C2-N1-C1'  | 6.87  | 126.35      | 118.80   |
| 1   | A     | 919  | U    | N1-C2-O2   | 6.85  | 127.59      | 122.80   |
| 34  | a     | 1494 | G    | N3-C4-C5   | -6.77 | 125.21      | 128.60   |
| 34  | a     | 1201 | A    | P-O3'-C3'  | 6.76  | 127.81      | 119.70   |
| 57  | x     | 35   | C    | N1-C2-O2   | 6.75  | 122.95      | 118.90   |
| 34  | a     | 611  | C    | N3-C2-O2   | -6.74 | 117.18      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 1022 | G    | P-O3'-C3' | 6.73  | 127.78      | 119.70   |
| 1   | A     | 192  | C    | N1-C2-O2  | 6.73  | 122.94      | 118.90   |
| 1   | A     | 2580 | U    | N3-C2-O2  | -6.72 | 117.49      | 122.20   |
| 34  | a     | 1297 | G    | P-O3'-C3' | 6.71  | 127.75      | 119.70   |
| 1   | A     | 2043 | C    | C2-N1-C1' | 6.71  | 126.18      | 118.80   |
| 1   | A     | 2072 | C    | C5-C6-N1  | 6.70  | 124.35      | 121.00   |
| 1   | A     | 1378 | A    | OP1-P-O3' | 6.70  | 119.93      | 105.20   |
| 2   | B     | 35   | C    | N3-C2-O2  | -6.66 | 117.23      | 121.90   |
| 1   | A     | 1914 | C    | N1-C2-O2  | 6.64  | 122.89      | 118.90   |
| 57  | x     | 67   | C    | N3-C2-O2  | -6.64 | 117.25      | 121.90   |
| 2   | B     | 31   | C    | C2-N1-C1' | 6.63  | 126.09      | 118.80   |
| 1   | A     | 1020 | A    | P-O3'-C3' | 6.62  | 127.64      | 119.70   |
| 1   | A     | 1956 | U    | N1-C2-O2  | 6.61  | 127.43      | 122.80   |
| 57  | x     | 67   | C    | C2-N1-C1' | 6.61  | 126.07      | 118.80   |
| 1   | A     | 2072 | C    | C6-N1-C2  | -6.57 | 117.67      | 120.30   |
| 2   | B     | 12   | C    | N3-C2-O2  | -6.54 | 117.32      | 121.90   |
| 1   | A     | 1917 | U    | C2-N1-C1' | 6.53  | 125.54      | 117.70   |
| 34  | a     | 439  | U    | N1-C2-O2  | 6.53  | 127.37      | 122.80   |
| 1   | A     | 2794 | C    | N1-C2-O2  | 6.52  | 122.81      | 118.90   |
| 13  | M     | 70   | ASP  | CB-CG-OD1 | 6.47  | 124.13      | 118.30   |
| 2   | B     | 35   | C    | C6-N1-C2  | -6.46 | 117.72      | 120.30   |
| 2   | B     | 12   | C    | C6-N1-C2  | -6.43 | 117.73      | 120.30   |
| 34  | a     | 1348 | U    | N3-C2-O2  | -6.43 | 117.70      | 122.20   |
| 1   | A     | 2457 | U    | N1-C2-O2  | 6.41  | 127.29      | 122.80   |
| 1   | A     | 1956 | U    | N3-C2-O2  | -6.38 | 117.73      | 122.20   |
| 1   | A     | 2636 | C    | N1-C2-O2  | 6.38  | 122.73      | 118.90   |
| 34  | a     | 1301 | U    | C2-N1-C1' | 6.37  | 125.34      | 117.70   |
| 34  | a     | 1132 | C    | N1-C2-O2  | 6.36  | 122.71      | 118.90   |
| 1   | A     | 2226 | C    | C6-N1-C2  | -6.34 | 117.76      | 120.30   |
| 34  | a     | 611  | C    | C2-N1-C1' | 6.34  | 125.78      | 118.80   |
| 1   | A     | 2704 | C    | N1-C2-O2  | 6.33  | 122.70      | 118.90   |
| 34  | a     | 644  | U    | N3-C2-O2  | -6.33 | 117.77      | 122.20   |
| 2   | B     | 26   | C    | N3-C2-O2  | -6.33 | 117.47      | 121.90   |
| 1   | A     | 1774 | C    | C6-N1-C2  | -6.31 | 117.78      | 120.30   |
| 1   | A     | 1917 | U    | N3-C2-O2  | -6.31 | 117.78      | 122.20   |
| 2   | B     | 17   | C    | C2-N1-C1' | 6.31  | 125.74      | 118.80   |
| 1   | A     | 114  | U    | C2-N1-C1' | 6.30  | 125.25      | 117.70   |
| 1   | A     | 1348 | C    | C6-N1-C2  | -6.29 | 117.78      | 120.30   |
| 34  | a     | 528  | C    | N1-C2-O2  | 6.29  | 122.67      | 118.90   |
| 2   | B     | 26   | C    | C2-N1-C1' | 6.27  | 125.70      | 118.80   |
| 34  | a     | 1348 | U    | C2-N1-C1' | 6.26  | 125.21      | 117.70   |
| 1   | A     | 1348 | C    | C2-N1-C1' | 6.25  | 125.67      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 919  | U    | N3-C2-O2  | -6.24 | 117.83      | 122.20   |
| 1   | A     | 752  | A    | OP2-P-O3' | 6.21  | 118.85      | 105.20   |
| 1   | A     | 1180 | U    | C2-N1-C1' | 6.21  | 125.15      | 117.70   |
| 1   | A     | 915  | C    | C2-N1-C1' | 6.20  | 125.62      | 118.80   |
| 1   | A     | 1917 | U    | N1-C2-O2  | 6.18  | 127.12      | 122.80   |
| 1   | A     | 2794 | C    | C6-N1-C2  | -6.17 | 117.83      | 120.30   |
| 1   | A     | 2214 | C    | N1-C2-O2  | 6.16  | 122.59      | 118.90   |
| 1   | A     | 2506 | U    | C5-C6-N1  | 6.16  | 125.78      | 122.70   |
| 34  | a     | 316  | C    | C2-N1-C1' | 6.14  | 125.55      | 118.80   |
| 37  | d     | 4    | LEU  | CA-CB-CG  | 6.14  | 129.41      | 115.30   |
| 1   | A     | 902  | C    | C2-N1-C1' | 6.13  | 125.55      | 118.80   |
| 1   | A     | 2072 | C    | N1-C2-O2  | 6.13  | 122.58      | 118.90   |
| 1   | A     | 1294 | U    | N1-C2-O2  | 6.12  | 127.08      | 122.80   |
| 34  | a     | 644  | U    | N1-C2-O2  | 6.10  | 127.07      | 122.80   |
| 1   | A     | 2457 | U    | N3-C2-O2  | -6.09 | 117.94      | 122.20   |
| 2   | B     | 11   | C    | N1-C2-O2  | 6.09  | 122.56      | 118.90   |
| 34  | a     | 1494 | G    | C4-N9-C1' | 6.09  | 134.42      | 126.50   |
| 1   | A     | 1086 | A    | C2-N3-C4  | 6.09  | 113.64      | 110.60   |
| 34  | a     | 1182 | G    | P-O3'-C3' | 6.09  | 127.00      | 119.70   |
| 34  | a     | 1494 | G    | N3-C4-N9  | 6.08  | 129.65      | 126.00   |
| 1   | A     | 2720 | U    | N3-C2-O2  | -6.08 | 117.94      | 122.20   |
| 1   | A     | 2286 | G    | P-O3'-C3' | 6.08  | 126.99      | 119.70   |
| 34  | a     | 989  | U    | N3-C2-O2  | -6.05 | 117.97      | 122.20   |
| 34  | a     | 697  | U    | N1-C2-O2  | 6.04  | 127.03      | 122.80   |
| 34  | a     | 85   | U    | P-O3'-C3' | 6.03  | 126.94      | 119.70   |
| 2   | B     | 3    | C    | P-O3'-C3' | 6.02  | 126.92      | 119.70   |
| 1   | A     | 1081 | U    | C2-N1-C1' | 6.01  | 124.92      | 117.70   |
| 1   | A     | 2703 | C    | C6-N1-C2  | -5.98 | 117.91      | 120.30   |
| 34  | a     | 936  | C    | N1-C2-O2  | 5.98  | 122.49      | 118.90   |
| 1   | A     | 1294 | U    | N3-C2-O2  | -5.97 | 118.02      | 122.20   |
| 1   | A     | 2605 | U    | C2-N1-C1' | 5.97  | 124.86      | 117.70   |
| 34  | a     | 1399 | C    | P-O3'-C3' | 5.96  | 126.85      | 119.70   |
| 1   | A     | 2506 | U    | C6-N1-C1' | -5.96 | 112.86      | 121.20   |
| 1   | A     | 1070 | A    | P-O3'-C3' | 5.93  | 126.82      | 119.70   |
| 1   | A     | 2474 | U    | N1-C2-O2  | 5.93  | 126.95      | 122.80   |
| 34  | a     | 611  | C    | C6-N1-C2  | -5.92 | 117.93      | 120.30   |
| 34  | a     | 269  | C    | C2-N1-C1' | 5.92  | 125.31      | 118.80   |
| 34  | a     | 1158 | C    | N1-C2-O2  | 5.92  | 122.45      | 118.90   |
| 1   | A     | 2580 | U    | N1-C2-O2  | 5.91  | 126.94      | 122.80   |
| 34  | a     | 1202 | U    | N1-C2-O2  | 5.91  | 126.94      | 122.80   |
| 1   | A     | 1349 | C    | C2-N1-C1' | 5.91  | 125.30      | 118.80   |
| 1   | A     | 143  | C    | C2-N1-C1' | 5.91  | 125.30      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 34  | a     | 960  | U    | P-O3'-C3' | 5.90  | 126.78      | 119.70   |
| 1   | A     | 20   | C    | N1-C2-O2  | 5.90  | 122.44      | 118.90   |
| 34  | a     | 936  | C    | N3-C2-O2  | -5.89 | 117.78      | 121.90   |
| 1   | A     | 51   | G    | P-O3'-C3' | 5.87  | 126.75      | 119.70   |
| 1   | A     | 1221 | C    | C2-N1-C1' | 5.85  | 125.23      | 118.80   |
| 1   | A     | 2192 | U    | C2-N1-C1' | 5.85  | 124.72      | 117.70   |
| 1   | A     | 20   | C    | C2-N1-C1' | 5.84  | 125.23      | 118.80   |
| 1   | A     | 985  | C    | C2-N1-C1' | 5.84  | 125.22      | 118.80   |
| 1   | A     | 1081 | U    | N1-C2-O2  | 5.83  | 126.88      | 122.80   |
| 1   | A     | 1940 | U    | P-O3'-C3' | 5.83  | 126.69      | 119.70   |
| 57  | x     | 67   | C    | C6-N1-C2  | -5.82 | 117.97      | 120.30   |
| 1   | A     | 2096 | C    | C2-N1-C1' | 5.80  | 125.18      | 118.80   |
| 1   | A     | 1314 | C    | C2-N1-C1' | 5.79  | 125.16      | 118.80   |
| 1   | A     | 2636 | C    | C2-N1-C1' | 5.78  | 125.16      | 118.80   |
| 1   | A     | 242  | G    | P-O3'-C3' | 5.78  | 126.64      | 119.70   |
| 2   | B     | 12   | C    | C2-N1-C1' | 5.77  | 125.15      | 118.80   |
| 1   | A     | 985  | C    | N1-C2-O2  | 5.76  | 122.36      | 118.90   |
| 1   | A     | 2605 | U    | N3-C2-O2  | -5.76 | 118.17      | 122.20   |
| 34  | a     | 440  | C    | N1-C2-O2  | 5.76  | 122.36      | 118.90   |
| 56  | w     | 313  | ASP  | C-N-CA    | 5.76  | 136.10      | 121.70   |
| 34  | a     | 439  | U    | C5-C6-N1  | 5.76  | 125.58      | 122.70   |
| 34  | a     | 1494 | G    | C2-N3-C4  | 5.75  | 114.78      | 111.90   |
| 34  | a     | 697  | U    | N3-C2-O2  | -5.74 | 118.18      | 122.20   |
| 1   | A     | 2504 | U    | C2-N1-C1' | 5.73  | 124.58      | 117.70   |
| 1   | A     | 2655 | G    | P-O3'-C3' | 5.73  | 126.57      | 119.70   |
| 1   | A     | 2666 | C    | N1-C2-O2  | 5.73  | 122.34      | 118.90   |
| 1   | A     | 372  | G    | P-O3'-C3' | 5.72  | 126.57      | 119.70   |
| 2   | B     | 30   | C    | N1-C2-O2  | 5.72  | 122.33      | 118.90   |
| 1   | A     | 1914 | C    | N3-C2-O2  | -5.71 | 117.90      | 121.90   |
| 1   | A     | 1348 | C    | C5-C6-N1  | 5.70  | 123.85      | 121.00   |
| 2   | B     | 25   | U    | N1-C2-O2  | 5.70  | 126.79      | 122.80   |
| 2   | B     | 26   | C    | C6-N1-C2  | -5.68 | 118.03      | 120.30   |
| 16  | P     | 113  | LEU  | CA-CB-CG  | 5.67  | 128.35      | 115.30   |
| 1   | A     | 859  | G    | P-O3'-C3' | 5.66  | 126.50      | 119.70   |
| 34  | a     | 1190 | G    | P-O3'-C3' | 5.66  | 126.50      | 119.70   |
| 34  | a     | 1520 | C    | C2-N1-C1' | 5.66  | 125.03      | 118.80   |
| 1   | A     | 353  | C    | C2-N1-C1' | 5.66  | 125.03      | 118.80   |
| 34  | a     | 438  | U    | P-O3'-C3' | 5.66  | 126.49      | 119.70   |
| 34  | a     | 1132 | C    | C2-N1-C1' | 5.66  | 125.02      | 118.80   |
| 1   | A     | 867  | C    | N3-C2-O2  | -5.66 | 117.94      | 121.90   |
| 34  | a     | 439  | U    | N3-C2-O2  | -5.65 | 118.24      | 122.20   |
| 1   | A     | 669  | G    | C4-N9-C1' | 5.65  | 133.85      | 126.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 2604 | U    | N1-C2-O2    | 5.65  | 126.75      | 122.80   |
| 2   | B     | 17   | C    | C6-N1-C2    | -5.65 | 118.04      | 120.30   |
| 1   | A     | 2457 | U    | O4'-C1'-N1  | 5.64  | 112.71      | 108.20   |
| 34  | a     | 358  | U    | N3-C2-O2    | -5.64 | 118.25      | 122.20   |
| 34  | a     | 1225 | A    | C4-N9-C1'   | 5.64  | 136.44      | 126.30   |
| 1   | A     | 353  | C    | N1-C2-O2    | 5.63  | 122.28      | 118.90   |
| 1   | A     | 2720 | U    | N1-C2-O2    | 5.62  | 126.74      | 122.80   |
| 34  | a     | 620  | C    | N1-C2-O2    | 5.62  | 122.27      | 118.90   |
| 34  | a     | 754  | C    | N1-C2-O2    | 5.62  | 122.27      | 118.90   |
| 34  | a     | 989  | U    | N1-C2-O2    | 5.62  | 126.73      | 122.80   |
| 1   | A     | 2566 | A    | P-O3'-C3'   | 5.62  | 126.44      | 119.70   |
| 55  | v     | 72   | PRO  | N-CA-CB     | 5.61  | 110.04      | 103.30   |
| 2   | B     | 31   | C    | N1-C2-O2    | 5.61  | 122.27      | 118.90   |
| 1   | A     | 2683 | C    | N1-C2-O2    | 5.61  | 122.27      | 118.90   |
| 34  | a     | 1202 | U    | N3-C2-O2    | -5.61 | 118.27      | 122.20   |
| 57  | x     | 74   | A    | C1'-C2'-O2' | 5.61  | 127.42      | 110.60   |
| 1   | A     | 2474 | U    | C2-N1-C1'   | 5.60  | 124.42      | 117.70   |
| 1   | A     | 2192 | U    | N1-C2-O2    | 5.60  | 126.72      | 122.80   |
| 34  | a     | 1347 | G    | P-O3'-C3'   | 5.59  | 126.41      | 119.70   |
| 34  | a     | 1432 | G    | P-O3'-C3'   | 5.59  | 126.41      | 119.70   |
| 57  | x     | 57   | C    | N3-C2-O2    | -5.58 | 117.99      | 121.90   |
| 1   | A     | 2617 | U    | N3-C2-O2    | -5.56 | 118.31      | 122.20   |
| 34  | a     | 1300 | G    | P-O3'-C3'   | 5.56  | 126.37      | 119.70   |
| 34  | a     | 340  | U    | N3-C2-O2    | -5.55 | 118.31      | 122.20   |
| 1   | A     | 2473 | U    | C5-C6-N1    | 5.55  | 125.48      | 122.70   |
| 1   | A     | 2474 | U    | N3-C2-O2    | -5.54 | 118.32      | 122.20   |
| 34  | a     | 1125 | U    | N1-C2-O2    | 5.54  | 126.68      | 122.80   |
| 1   | A     | 955  | U    | C6-N1-C1'   | -5.53 | 113.45      | 121.20   |
| 1   | A     | 2457 | U    | C5-C4-O4    | 5.53  | 129.22      | 125.90   |
| 57  | x     | 35   | C    | C2-N1-C1'   | 5.53  | 124.88      | 118.80   |
| 1   | A     | 2192 | U    | N3-C2-O2    | -5.53 | 118.33      | 122.20   |
| 1   | A     | 2179 | C    | N1-C2-O2    | 5.52  | 122.21      | 118.90   |
| 34  | a     | 754  | C    | C6-N1-C1'   | -5.52 | 114.18      | 120.80   |
| 1   | A     | 2739 | U    | N1-C2-O2    | 5.51  | 126.66      | 122.80   |
| 1   | A     | 2178 | C    | N1-C2-O2    | 5.51  | 122.21      | 118.90   |
| 57  | x     | 35   | C    | N3-C2-O2    | -5.51 | 118.04      | 121.90   |
| 34  | a     | 439  | U    | C2-N1-C1'   | 5.50  | 124.30      | 117.70   |
| 1   | A     | 192  | C    | N3-C2-O2    | -5.49 | 118.06      | 121.90   |
| 1   | A     | 1306 | C    | C2-N1-C1'   | 5.49  | 124.83      | 118.80   |
| 1   | A     | 1914 | C    | C5-C6-N1    | 5.49  | 123.74      | 121.00   |
| 1   | A     | 2703 | C    | C2-N1-C1'   | 5.48  | 124.83      | 118.80   |
| 2   | B     | 31   | C    | C6-N1-C2    | -5.48 | 118.11      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 2739 | U    | N3-C2-O2  | -5.47 | 118.37      | 122.20   |
| 34  | a     | 283  | U    | N1-C2-O2  | 5.47  | 126.63      | 122.80   |
| 1   | A     | 1818 | U    | C2-N1-C1' | 5.46  | 124.26      | 117.70   |
| 57  | x     | 35   | C    | C6-N1-C2  | -5.46 | 118.11      | 120.30   |
| 34  | a     | 440  | C    | C6-N1-C2  | -5.46 | 118.12      | 120.30   |
| 34  | a     | 316  | C    | C6-N1-C2  | -5.46 | 118.12      | 120.30   |
| 34  | a     | 1138 | G    | C4-N9-C1' | 5.46  | 133.59      | 126.50   |
| 34  | a     | 340  | U    | N1-C2-O2  | 5.45  | 126.62      | 122.80   |
| 1   | A     | 837  | C    | N3-C2-O2  | -5.45 | 118.08      | 121.90   |
| 1   | A     | 166  | U    | N1-C2-O2  | 5.45  | 126.62      | 122.80   |
| 1   | A     | 1839 | G    | C4-N9-C1' | 5.44  | 133.57      | 126.50   |
| 1   | A     | 1079 | C    | N1-C2-O2  | 5.44  | 122.16      | 118.90   |
| 1   | A     | 2300 | C    | C2-N1-C1' | 5.43  | 124.78      | 118.80   |
| 1   | A     | 479  | A    | P-O3'-C3' | 5.43  | 126.22      | 119.70   |
| 1   | A     | 1818 | U    | N1-C2-O2  | 5.42  | 126.60      | 122.80   |
| 1   | A     | 206  | U    | N1-C2-O2  | 5.42  | 126.59      | 122.80   |
| 1   | A     | 919  | U    | C2-N1-C1' | 5.41  | 124.19      | 117.70   |
| 34  | a     | 269  | C    | C6-N1-C2  | -5.41 | 118.14      | 120.30   |
| 1   | A     | 897  | C    | N1-C2-O2  | 5.41  | 122.15      | 118.90   |
| 37  | d     | 190  | LEU  | CA-CB-CG  | 5.41  | 127.74      | 115.30   |
| 1   | A     | 2063 | C    | C5-C6-N1  | 5.41  | 123.70      | 121.00   |
| 57  | x     | 25   | U    | OP1-P-O3' | 5.40  | 117.08      | 105.20   |
| 1   | A     | 234  | U    | N3-C2-O2  | -5.39 | 118.42      | 122.20   |
| 1   | A     | 2769 | U    | N1-C2-O2  | 5.39  | 126.57      | 122.80   |
| 1   | A     | 1188 | U    | N1-C2-O2  | 5.38  | 126.57      | 122.80   |
| 1   | A     | 1349 | C    | C6-N1-C2  | -5.38 | 118.15      | 120.30   |
| 1   | A     | 166  | U    | N3-C2-O2  | -5.38 | 118.43      | 122.20   |
| 1   | A     | 137  | U    | N3-C2-O2  | -5.38 | 118.44      | 122.20   |
| 1   | A     | 444  | C    | N1-C2-O2  | 5.37  | 122.12      | 118.90   |
| 34  | a     | 961  | U    | N1-C2-O2  | 5.37  | 126.56      | 122.80   |
| 57  | x     | 25   | U    | N1-C2-O2  | 5.37  | 126.56      | 122.80   |
| 1   | A     | 1760 | C    | N1-C2-O2  | 5.36  | 122.12      | 118.90   |
| 1   | A     | 2884 | U    | C2-N1-C1' | 5.36  | 124.13      | 117.70   |
| 34  | a     | 1262 | C    | N1-C2-O2  | 5.36  | 122.12      | 118.90   |
| 1   | A     | 1086 | A    | N3-C4-N9  | 5.36  | 131.69      | 127.40   |
| 1   | A     | 2552 | U    | C2-N1-C1' | 5.36  | 124.13      | 117.70   |
| 2   | B     | 11   | C    | C6-N1-C2  | -5.35 | 118.16      | 120.30   |
| 1   | A     | 20   | C    | C6-N1-C2  | -5.35 | 118.16      | 120.30   |
| 1   | A     | 1086 | A    | C4-N9-C1' | 5.34  | 135.92      | 126.30   |
| 1   | A     | 1294 | U    | C2-N1-C1' | 5.34  | 124.11      | 117.70   |
| 34  | a     | 1125 | U    | N3-C2-O2  | -5.34 | 118.46      | 122.20   |
| 1   | A     | 417  | C    | C2-N1-C1' | 5.34  | 124.67      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 2615 | U    | N3-C2-O2   | -5.34 | 118.46      | 122.20   |
| 2   | B     | 11   | C    | N3-C2-O2   | -5.34 | 118.17      | 121.90   |
| 1   | A     | 2254 | C    | N1-C2-O2   | 5.33  | 122.10      | 118.90   |
| 1   | A     | 2605 | U    | N1-C2-O2   | 5.32  | 126.52      | 122.80   |
| 2   | B     | 3    | C    | OP1-P-O3'  | 5.32  | 116.91      | 105.20   |
| 1   | A     | 897  | C    | P-O3'-C3'  | 5.32  | 126.08      | 119.70   |
| 2   | B     | 25   | U    | N3-C2-O2   | -5.31 | 118.48      | 122.20   |
| 30  | 3     | 61   | LEU  | CA-CB-CG   | 5.31  | 127.52      | 115.30   |
| 1   | A     | 2342 | C    | N3-C2-O2   | -5.31 | 118.19      | 121.90   |
| 57  | x     | 25   | U    | P-O3'-C3'  | 5.31  | 126.07      | 119.70   |
| 1   | A     | 902  | C    | N1-C2-O2   | 5.30  | 122.08      | 118.90   |
| 1   | A     | 1911 | U    | C2-N1-C1'  | 5.30  | 124.06      | 117.70   |
| 1   | A     | 2473 | U    | C6-N1-C2   | -5.29 | 117.83      | 121.00   |
| 1   | A     | 1880 | U    | N3-C2-O2   | -5.28 | 118.50      | 122.20   |
| 1   | A     | 634  | C    | N1-C2-O2   | 5.27  | 122.06      | 118.90   |
| 1   | A     | 1818 | U    | N3-C2-O2   | -5.27 | 118.51      | 122.20   |
| 1   | A     | 985  | C    | C6-N1-C2   | -5.26 | 118.20      | 120.30   |
| 1   | A     | 1812 | U    | C2-N1-C1'  | 5.25  | 124.00      | 117.70   |
| 1   | A     | 2615 | U    | N1-C2-O2   | 5.25  | 126.47      | 122.80   |
| 1   | A     | 1893 | C    | C6-N1-C2   | -5.24 | 118.20      | 120.30   |
| 1   | A     | 1812 | U    | N3-C2-O2   | -5.24 | 118.53      | 122.20   |
| 1   | A     | 206  | U    | N3-C2-O2   | -5.24 | 118.53      | 122.20   |
| 1   | A     | 2617 | U    | N1-C2-O2   | 5.24  | 126.47      | 122.80   |
| 34  | a     | 469  | C    | N1-C2-O2   | 5.23  | 122.04      | 118.90   |
| 1   | A     | 2460 | U    | N1-C2-O2   | 5.22  | 126.45      | 122.80   |
| 1   | A     | 114  | U    | N1-C2-O2   | 5.22  | 126.45      | 122.80   |
| 1   | A     | 2506 | U    | C6-N1-C2   | -5.21 | 117.87      | 121.00   |
| 34  | a     | 1225 | A    | N3-C4-N9   | 5.20  | 131.56      | 127.40   |
| 57  | x     | 26   | C    | C6-N1-C2   | -5.20 | 118.22      | 120.30   |
| 1   | A     | 353  | C    | C6-N1-C2   | -5.20 | 118.22      | 120.30   |
| 1   | A     | 2752 | C    | N1-C2-O2   | 5.19  | 122.02      | 118.90   |
| 34  | a     | 1203 | C    | C2-N1-C1'  | 5.19  | 124.50      | 118.80   |
| 57  | x     | 74   | A    | N9-C1'-C2' | -5.19 | 106.30      | 112.00   |
| 1   | A     | 1417 | C    | C2-N1-C1'  | 5.18  | 124.50      | 118.80   |
| 34  | a     | 1469 | C    | N1-C2-O2   | 5.18  | 122.01      | 118.90   |
| 1   | A     | 1321 | A    | C2-N3-C4   | 5.18  | 113.19      | 110.60   |
| 1   | A     | 2043 | C    | C6-N1-C2   | -5.18 | 118.23      | 120.30   |
| 34  | a     | 1086 | U    | N1-C2-O2   | 5.16  | 126.41      | 122.80   |
| 1   | A     | 2226 | C    | C5-C6-N1   | 5.16  | 123.58      | 121.00   |
| 1   | A     | 1079 | C    | N3-C2-O2   | -5.16 | 118.29      | 121.90   |
| 1   | A     | 1306 | C    | N1-C2-O2   | 5.15  | 121.99      | 118.90   |
| 1   | A     | 837  | C    | N1-C2-O2   | 5.15  | 121.99      | 118.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 2703 | C    | N1-C2-O2   | 5.15  | 121.99      | 118.90   |
| 34  | a     | 1138 | G    | N3-C4-C5   | -5.15 | 126.03      | 128.60   |
| 1   | A     | 758  | C    | N1-C2-O2   | 5.14  | 121.99      | 118.90   |
| 1   | A     | 2590 | A    | N1-C6-N6   | -5.14 | 115.51      | 118.60   |
| 34  | a     | 283  | U    | N3-C2-O2   | -5.14 | 118.60      | 122.20   |
| 1   | A     | 1398 | C    | C2-N1-C1'  | 5.13  | 124.45      | 118.80   |
| 1   | A     | 2504 | U    | N1-C2-O2   | 5.13  | 126.39      | 122.80   |
| 1   | A     | 62   | U    | C2-N1-C1'  | 5.13  | 123.86      | 117.70   |
| 1   | A     | 137  | U    | N1-C2-O2   | 5.13  | 126.39      | 122.80   |
| 34  | a     | 440  | C    | C2-N1-C1'  | 5.13  | 124.44      | 118.80   |
| 1   | A     | 484  | C    | C6-N1-C2   | -5.12 | 118.25      | 120.30   |
| 1   | A     | 2076 | U    | C2-N1-C1'  | 5.11  | 123.83      | 117.70   |
| 1   | A     | 2636 | C    | C6-N1-C2   | -5.11 | 118.25      | 120.30   |
| 34  | a     | 1399 | C    | OP2-P-O3'  | 5.11  | 116.44      | 105.20   |
| 1   | A     | 955  | U    | O4'-C1'-N1 | 5.11  | 112.28      | 108.20   |
| 2   | B     | 47   | C    | N1-C2-O2   | 5.11  | 121.96      | 118.90   |
| 1   | A     | 1839 | G    | N3-C4-N9   | 5.10  | 129.06      | 126.00   |
| 1   | A     | 1880 | U    | C2-N1-C1'  | 5.10  | 123.82      | 117.70   |
| 34  | a     | 154  | U    | N3-C2-O2   | -5.10 | 118.63      | 122.20   |
| 1   | A     | 550  | C    | N1-C2-O2   | 5.09  | 121.96      | 118.90   |
| 34  | a     | 316  | C    | N1-C2-O2   | 5.09  | 121.95      | 118.90   |
| 34  | a     | 893  | C    | N1-C2-O2   | 5.09  | 121.95      | 118.90   |
| 1   | A     | 234  | U    | N1-C2-O2   | 5.08  | 126.36      | 122.80   |
| 2   | B     | 17   | C    | C5-C6-N1   | 5.08  | 123.54      | 121.00   |
| 2   | B     | 66   | A    | P-O3'-C3'  | 5.08  | 125.80      | 119.70   |
| 1   | A     | 417  | C    | C5-C6-N1   | 5.08  | 123.54      | 121.00   |
| 34  | a     | 536  | C    | C6-N1-C2   | -5.08 | 118.27      | 120.30   |
| 2   | B     | 30   | C    | C6-N1-C2   | -5.07 | 118.27      | 120.30   |
| 34  | a     | 1158 | C    | N3-C2-O2   | -5.07 | 118.35      | 121.90   |
| 1   | A     | 1892 | C    | N1-C2-O2   | 5.06  | 121.94      | 118.90   |
| 34  | a     | 528  | C    | N3-C2-O2   | -5.05 | 118.36      | 121.90   |
| 1   | A     | 1376 | C    | C2-N1-C1'  | 5.05  | 124.35      | 118.80   |
| 1   | A     | 1880 | U    | N1-C2-O2   | 5.05  | 126.33      | 122.80   |
| 1   | A     | 2456 | C    | C6-N1-C2   | -5.05 | 118.28      | 120.30   |
| 34  | a     | 1314 | C    | N1-C2-O2   | 5.05  | 121.93      | 118.90   |
| 1   | A     | 2043 | C    | C5-C6-N1   | 5.04  | 123.52      | 121.00   |
| 34  | a     | 536  | C    | C5-C6-N1   | 5.04  | 123.52      | 121.00   |
| 34  | a     | 805  | C    | C6-N1-C2   | -5.04 | 118.28      | 120.30   |
| 1   | A     | 669  | G    | N3-C4-N9   | 5.04  | 129.02      | 126.00   |
| 1   | A     | 2063 | C    | C6-N1-C1'  | -5.03 | 114.77      | 120.80   |
| 1   | A     | 1945 | G    | C4-N9-C1'  | 5.02  | 133.03      | 126.50   |
| 34  | a     | 961  | U    | N3-C2-O2   | -5.02 | 118.68      | 122.20   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 34  | a     | 1132 | C    | N3-C2-O2  | -5.02 | 118.39      | 121.90   |
| 1   | A     | 2769 | U    | N3-C2-O2  | -5.02 | 118.69      | 122.20   |
| 57  | x     | 25   | U    | N3-C2-O2  | -5.01 | 118.69      | 122.20   |
| 34  | a     | 805  | C    | C2-N1-C1' | 5.01  | 124.31      | 118.80   |
| 1   | A     | 2460 | U    | N3-C2-O2  | -5.01 | 118.70      | 122.20   |
| 57  | x     | 57   | C    | N1-C2-O2  | 5.01  | 121.90      | 118.90   |
| 1   | A     | 1812 | U    | N1-C2-O2  | 5.00  | 126.30      | 122.80   |

There are no chirality outliers.

All (27) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 30  | 3     | 27  | ASN  | Peptide   |
| 30  | 3     | 30  | HIS  | Peptide   |
| 32  | 5     | 80  | THR  | Peptide   |
| 6   | F     | 173 | ASP  | Peptide   |
| 6   | F     | 174 | PHE  | Peptide   |
| 7   | G     | 118 | ALA  | Peptide   |
| 7   | G     | 45  | ALA  | Peptide   |
| 7   | G     | 46  | ASP  | Peptide   |
| 11  | K     | 88  | ASN  | Peptide   |
| 13  | M     | 57  | VAL  | Peptide   |
| 18  | R     | 53  | PHE  | Peptide   |
| 21  | U     | 88  | ASP  | Peptide   |
| 35  | b     | 15  | PHE  | Peptide   |
| 35  | b     | 16  | GLY  | Peptide   |
| 35  | b     | 18  | GLN  | Peptide   |
| 38  | e     | 121 | ASN  | Peptide   |
| 39  | f     | 53  | LYS  | Peptide   |
| 39  | f     | 95  | ALA  | Peptide   |
| 42  | i     | 90  | ASP  | Peptide   |
| 43  | j     | 57  | VAL  | Peptide   |
| 45  | l     | 101 | LEU  | Peptide   |
| 46  | m     | 4   | ALA  | Peptide   |
| 50  | q     | 68  | LYS  | Peptide   |
| 55  | v     | 320 | HIS  | Mainchain |
| 56  | w     | 17  | ALA  | Peptide   |
| 56  | w     | 314 | ARG  | Peptide   |
| 56  | w     | 76  | GLN  | Peptide   |

## 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   | A     | 62153 | 0        | 31259    | 451     | 0            |
| 2   | B     | 2572  | 0        | 1302     | 19      | 0            |
| 3   | C     | 2082  | 0        | 2157     | 37      | 0            |
| 4   | D     | 1565  | 0        | 1616     | 19      | 0            |
| 5   | E     | 1552  | 0        | 1619     | 20      | 0            |
| 6   | F     | 1410  | 0        | 1447     | 17      | 0            |
| 7   | G     | 1323  | 0        | 1374     | 7       | 0            |
| 8   | H     | 1111  | 0        | 1148     | 13      | 0            |
| 9   | I     | 1032  | 0        | 1088     | 11      | 0            |
| 10  | J     | 1129  | 0        | 1162     | 13      | 0            |
| 11  | K     | 938   | 0        | 1012     | 12      | 0            |
| 12  | L     | 1045  | 0        | 1117     | 14      | 0            |
| 13  | M     | 1074  | 0        | 1157     | 12      | 0            |
| 14  | N     | 960   | 0        | 1000     | 11      | 0            |
| 15  | O     | 892   | 0        | 923      | 10      | 0            |
| 16  | P     | 917   | 0        | 965      | 13      | 0            |
| 17  | Q     | 947   | 0        | 1022     | 10      | 0            |
| 18  | R     | 816   | 0        | 839      | 11      | 0            |
| 19  | S     | 857   | 0        | 922      | 8       | 0            |
| 20  | T     | 738   | 0        | 807      | 13      | 0            |
| 21  | U     | 779   | 0        | 834      | 6       | 0            |
| 22  | V     | 753   | 0        | 780      | 7       | 0            |
| 23  | W     | 575   | 0        | 592      | 3       | 0            |
| 24  | X     | 625   | 0        | 655      | 9       | 0            |
| 25  | Y     | 509   | 0        | 543      | 7       | 0            |
| 26  | Z     | 449   | 0        | 491      | 4       | 0            |
| 27  | 0     | 444   | 0        | 461      | 6       | 0            |
| 28  | 1     | 409   | 0        | 440      | 3       | 0            |
| 29  | 2     | 377   | 0        | 418      | 12      | 0            |
| 30  | 3     | 504   | 0        | 574      | 13      | 0            |
| 31  | 4     | 302   | 0        | 343      | 5       | 0            |
| 32  | 5     | 988   | 0        | 1025     | 14      | 0            |
| 33  | 7     | 151   | 0        | 76       | 3       | 0            |
| 34  | a     | 33016 | 0        | 16616    | 0       | 0            |
| 35  | b     | 1704  | 0        | 1732     | 0       | 0            |
| 36  | c     | 1624  | 0        | 1699     | 0       | 0            |
| 37  | d     | 1643  | 0        | 1710     | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 38  | e     | 1141   | 0        | 1170     | 0       | 0            |
| 39  | f     | 817    | 0        | 808      | 0       | 0            |
| 40  | g     | 1181   | 0        | 1240     | 0       | 0            |
| 41  | h     | 979    | 0        | 1034     | 0       | 0            |
| 42  | i     | 1022   | 0        | 1070     | 0       | 0            |
| 43  | j     | 786    | 0        | 828      | 0       | 0            |
| 44  | k     | 869    | 0        | 878      | 0       | 0            |
| 45  | l     | 955    | 0        | 1019     | 0       | 0            |
| 46  | m     | 883    | 0        | 944      | 0       | 0            |
| 47  | n     | 799    | 0        | 841      | 0       | 0            |
| 48  | o     | 714    | 0        | 737      | 0       | 0            |
| 49  | p     | 649    | 0        | 666      | 0       | 0            |
| 50  | q     | 648    | 0        | 691      | 0       | 0            |
| 51  | r     | 504    | 0        | 502      | 0       | 0            |
| 52  | s     | 637    | 0        | 665      | 0       | 0            |
| 53  | t     | 665    | 0        | 714      | 0       | 0            |
| 54  | u     | 495    | 0        | 486      | 0       | 0            |
| 55  | v     | 2436   | 0        | 2125     | 0       | 0            |
| 56  | w     | 3923   | 0        | 3916     | 0       | 0            |
| 57  | x     | 1640   | 0        | 837      | 0       | 0            |
| 58  | z     | 120    | 0        | 128      | 0       | 0            |
| 59  | w     | 32     | 0        | 14       | 0       | 0            |
| All | All   | 151860 | 0        | 104238   | 696     | 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 6.

All (696) 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) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:745:G:N7   | 1:A:746:U:C5   | 2.25                     | 1.04              |
| 1:A:1476:U:H3  | 1:A:1515:A:H62 | 0.99                     | 0.96              |
| 1:A:545:U:H3   | 1:A:548:G:H1   | 1.00                     | 0.93              |
| 1:A:2475:C:H42 | 1:A:2529:G:N2  | 1.66                     | 0.93              |
| 1:A:306:U:H3   | 1:A:310:A:H62  | 0.95                     | 0.91              |
| 1:A:2028:U:H3  | 1:A:2033:A:H62 | 1.12                     | 0.90              |
| 1:A:2457:U:H5  | 1:A:2494:G:H1  | 0.90                     | 0.87              |
| 1:A:2475:C:H42 | 1:A:2529:G:H22 | 1.20                     | 0.86              |
| 1:A:306:U:H3   | 1:A:310:A:N6   | 1.75                     | 0.83              |
| 1:A:244:A:H62  | 1:A:254:G:H21  | 1.28                     | 0.80              |
| 1:A:745:G:C5   | 1:A:746:U:C6   | 2.69                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:593:U:H3     | 1:A:664:G:H1     | 1.29                     | 0.80              |
| 1:A:2475:C:N4    | 1:A:2529:G:H22   | 1.80                     | 0.79              |
| 1:A:2457:U:H5    | 1:A:2494:G:N1    | 1.75                     | 0.79              |
| 1:A:2508:G:N1    | 1:A:2580:U:O4    | 2.16                     | 0.77              |
| 1:A:2514:U:H3    | 1:A:2570:G:H1    | 1.35                     | 0.74              |
| 1:A:745:G:N7     | 1:A:746:U:C6     | 2.57                     | 0.73              |
| 23:W:61:GLY:HA3  | 23:W:79:GLU:O    | 1.89                     | 0.73              |
| 1:A:600:G:H1     | 1:A:657:U:H3     | 1.38                     | 0.69              |
| 1:A:1476:U:H3    | 1:A:1515:A:N6    | 1.84                     | 0.69              |
| 1:A:955:U:C5     | 1:A:962:G:N1     | 2.58                     | 0.69              |
| 1:A:2457:U:O4    | 1:A:2494:G:O6    | 2.13                     | 0.67              |
| 1:A:1912:A:N7    | 1:A:1917:U:O4    | 2.27                     | 0.67              |
| 2:B:78:A:H62     | 2:B:98:G:H21     | 1.40                     | 0.67              |
| 16:P:59:THR:HG22 | 16:P:72:VAL:HG12 | 1.77                     | 0.67              |
| 1:A:78:U:H3      | 1:A:108:G:H1     | 1.43                     | 0.65              |
| 1:A:2508:G:C6    | 1:A:2580:U:O4    | 2.49                     | 0.65              |
| 1:A:1418:G:N2    | 1:A:1579:A:N7    | 2.46                     | 0.64              |
| 1:A:955:U:H5     | 1:A:962:G:H1     | 1.43                     | 0.64              |
| 1:A:1666:G:H4'   | 11:K:6:THR:HG23  | 1.78                     | 0.64              |
| 1:A:745:G:C5     | 1:A:746:U:C5     | 2.86                     | 0.63              |
| 14:N:28:LEU:HD23 | 14:N:48:VAL:HG21 | 1.81                     | 0.63              |
| 1:A:955:U:H5     | 1:A:962:G:N1     | 1.96                     | 0.63              |
| 1:A:1687:G:H21   | 1:A:1701:A:H62   | 1.46                     | 0.63              |
| 1:A:1433:A:H61   | 1:A:1560:G:H1    | 1.44                     | 0.62              |
| 1:A:244:A:H62    | 1:A:254:G:N2     | 1.97                     | 0.62              |
| 1:A:2508:G:O6    | 1:A:2580:U:O4    | 2.18                     | 0.62              |
| 1:A:1046:A:H62   | 32:5:4:ASN:HD21  | 1.48                     | 0.61              |
| 1:A:2028:U:H3    | 1:A:2033:A:N6    | 1.92                     | 0.61              |
| 1:A:306:U:O4     | 1:A:310:A:N7     | 2.34                     | 0.61              |
| 1:A:745:G:C6     | 1:A:746:U:C6     | 2.89                     | 0.61              |
| 1:A:2514:U:H5''  | 10:J:81:ILE:HD11 | 1.83                     | 0.60              |
| 22:V:64:VAL:HG22 | 22:V:69:GLU:HG2  | 1.83                     | 0.60              |
| 2:B:78:A:H62     | 2:B:98:G:N2      | 1.98                     | 0.60              |
| 4:D:34:VAL:HA    | 4:D:50:VAL:HG12  | 1.83                     | 0.60              |
| 1:A:955:U:O4     | 1:A:962:G:O6     | 2.20                     | 0.60              |
| 19:S:82:MET:HB2  | 19:S:98:LYS:HB2  | 1.83                     | 0.60              |
| 1:A:1081:U:H4'   | 9:I:123:ALA:HB1  | 1.84                     | 0.60              |
| 1:A:1252:G:N2    | 17:Q:32:ARG:O    | 2.35                     | 0.60              |
| 1:A:818:G:H21    | 1:A:1189:A:H62   | 1.47                     | 0.60              |
| 20:T:8:LEU:HA    | 20:T:50:LEU:HD21 | 1.84                     | 0.60              |
| 6:F:62:GLN:HE22  | 6:F:90:LEU:HB3   | 1.66                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:2656:U:O2    | 1:A:2665:A:N7    | 2.35                     | 0.60              |
| 1:A:488:G:H22    | 1:A:491:G:H5''   | 1.66                     | 0.59              |
| 8:H:39:ALA:HA    | 8:H:43:ASN:HB2   | 1.84                     | 0.59              |
| 1:A:1093:G:H21   | 1:A:1098:A:H62   | 1.48                     | 0.59              |
| 29:2:24:THR:HG23 | 29:2:27:GLY:H    | 1.67                     | 0.59              |
| 32:5:58:THR:HG21 | 32:5:82:ILE:H    | 1.68                     | 0.59              |
| 1:A:1940:U:OP1   | 1:A:2603:G:N2    | 2.34                     | 0.59              |
| 1:A:2296:U:OP2   | 15:O:9:ARG:NH2   | 2.35                     | 0.59              |
| 1:A:1798:U:H5''  | 3:C:257:ARG:HB2  | 1.84                     | 0.59              |
| 5:E:146:VAL:HG12 | 5:E:185:LYS:HB2  | 1.83                     | 0.59              |
| 1:A:629:G:N3     | 1:A:639:U:O2'    | 2.34                     | 0.59              |
| 1:A:2748:A:H5'   | 7:G:3:VAL:HG21   | 1.85                     | 0.59              |
| 1:A:281:C:H42    | 1:A:359:G:H1     | 1.50                     | 0.59              |
| 1:A:538:A:H4'    | 10:J:7:LYS:HG2   | 1.85                     | 0.59              |
| 2:B:72:G:H21     | 2:B:104:A:H62    | 1.51                     | 0.59              |
| 1:A:463:G:N2     | 1:A:466:A:OP2    | 2.35                     | 0.59              |
| 1:A:1153:C:OP1   | 17:Q:91:ARG:NH2  | 2.35                     | 0.58              |
| 15:O:40:ILE:HG12 | 15:O:47:VAL:HG12 | 1.85                     | 0.58              |
| 1:A:1060:U:H5'   | 1:A:1062:G:H5'   | 1.84                     | 0.58              |
| 1:A:674:G:O6     | 1:A:716:A:N1     | 104.06                   | 0.58              |
| 1:A:839:U:H3     | 1:A:939:G:H1     | 1.51                     | 0.58              |
| 1:A:1862:G:H1    | 1:A:1880:U:H3    | 1.50                     | 0.58              |
| 2:B:30:C:H1'     | 2:B:57:A:H61     | 1.69                     | 0.58              |
| 2:B:79:G:N7      | 22:V:14:LYS:NZ   | 2.52                     | 0.57              |
| 1:A:585:G:H21    | 1:A:1254:A:H62   | 1.52                     | 0.57              |
| 1:A:2743:U:OP2   | 1:A:2755:C:N4    | 2.38                     | 0.57              |
| 1:A:1309:G:H5''  | 29:2:9:VAL:HG23  | 1.87                     | 0.57              |
| 9:I:11:GLN:NE2   | 9:I:54:ILE:O     | 2.38                     | 0.57              |
| 1:A:2185:U:H2'   | 1:A:2186:G:H8    | 1.69                     | 0.57              |
| 30:3:32:LEU:HD23 | 30:3:35:LYS:HD2  | 1.86                     | 0.57              |
| 1:A:1450:G:H21   | 1:A:1452:G:H1    | 1.53                     | 0.57              |
| 26:Z:8:GLN:HB2   | 26:Z:28:LEU:HD13 | 1.87                     | 0.57              |
| 1:A:1986:C:H2'   | 1:A:1987:A:H8    | 1.70                     | 0.57              |
| 1:A:1992:G:N2    | 1:A:1996:C:O2'   | 2.37                     | 0.57              |
| 1:A:962:G:O2'    | 1:A:2250:G:N2    | 2.38                     | 0.57              |
| 5:E:117:ARG:NH2  | 5:E:183:PHE:O    | 2.38                     | 0.57              |
| 1:A:587:C:O2     | 12:L:33:ARG:NH1  | 2.38                     | 0.57              |
| 24:X:6:VAL:HG21  | 24:X:58:ILE:HD11 | 1.86                     | 0.57              |
| 1:A:698:C:O2'    | 1:A:734:A:N6     | 2.35                     | 0.57              |
| 4:D:179:ARG:HB3  | 4:D:188:LEU:HD12 | 1.86                     | 0.57              |
| 1:A:2515:C:H2'   | 1:A:2516:A:H8    | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:2692:G:H1'   | 1:A:2847:U:H1'   | 1.87                     | 0.56              |
| 1:A:605:G:H1'    | 1:A:657:U:H1'    | 1.87                     | 0.56              |
| 1:A:2028:U:O4    | 1:A:2033:A:N7    | 2.38                     | 0.56              |
| 6:F:23:SER:HB3   | 6:F:26:GLN:HG3   | 1.86                     | 0.56              |
| 20:T:23:ALA:HB1  | 20:T:29:THR:HB   | 1.87                     | 0.56              |
| 1:A:1422:G:H5'   | 11:K:48:PRO:HG3  | 98.75                    | 0.56              |
| 1:A:2291:U:H1'   | 1:A:2374:C:H1'   | 1.88                     | 0.56              |
| 1:A:605:G:OP1    | 5:E:99:LYS:NZ    | 2.38                     | 0.56              |
| 23:W:33:ILE:HG22 | 23:W:34:VAL:HG23 | 1.88                     | 0.56              |
| 1:A:1476:U:O4    | 1:A:1515:A:N7    | 2.39                     | 0.56              |
| 6:F:134:GLN:NE2  | 6:F:149:ARG:O    | 2.38                     | 0.56              |
| 3:C:92:LEU:HD11  | 3:C:100:ARG:HB3  | 1.86                     | 0.56              |
| 1:A:605:G:N3     | 1:A:657:U:O2'    | 2.38                     | 0.56              |
| 17:Q:43:GLN:HE21 | 18:R:77:PHE:HB3  | 1.71                     | 0.56              |
| 21:U:33:VAL:HG13 | 21:U:66:VAL:HG22 | 1.87                     | 0.56              |
| 1:A:1500:G:H4'   | 3:C:100:ARG:HH12 | 1.71                     | 0.56              |
| 1:A:2062:A:H62   | 1:A:2503:A:H62   | 1.53                     | 0.56              |
| 7:G:88:LEU:HG    | 7:G:161:VAL:HG22 | 1.87                     | 0.55              |
| 22:V:42:LEU:HD13 | 22:V:47:VAL:HG21 | 1.86                     | 0.55              |
| 27:O:30:ASP:HB3  | 27:O:34:GLY:H    | 1.71                     | 0.55              |
| 1:A:318:C:H2'    | 1:A:319:G:H8     | 1.72                     | 0.55              |
| 3:C:51:ARG:HH22  | 3:C:246:PRO:HG2  | 1.70                     | 0.55              |
| 1:A:2095:A:OP1   | 8:H:11:ASN:ND2   | 2.40                     | 0.55              |
| 24:X:39:VAL:HG12 | 24:X:42:GLU:H    | 1.70                     | 0.55              |
| 3:C:143:VAL:HB   | 3:C:153:LEU:HB2  | 1.87                     | 0.55              |
| 1:A:682:G:O2'    | 29:2:33:ARG:NH1  | 2.40                     | 0.55              |
| 1:A:2314:A:OP1   | 6:F:87:LYS:NZ    | 2.39                     | 0.55              |
| 1:A:1668:A:N3    | 1:A:1670:C:N4    | 2.55                     | 0.55              |
| 1:A:2893:A:H5''  | 1:A:2894:G:H5'   | 1.89                     | 0.55              |
| 1:A:406:G:H5'    | 4:D:4:LEU:HD22   | 165.75                   | 0.55              |
| 7:G:94:ARG:HB2   | 7:G:105:SER:HB2  | 1.88                     | 0.55              |
| 1:A:686:U:O4     | 29:2:12:ARG:NH2  | 2.39                     | 0.55              |
| 1:A:911:A:N6     | 13:M:11:LYS:O    | 2.37                     | 0.55              |
| 1:A:144:A:H4'    | 20:T:2:ILE:HD11  | 1.89                     | 0.55              |
| 1:A:514:A:N3     | 1:A:581:C:O2'    | 2.37                     | 0.55              |
| 1:A:647:G:N2     | 1:A:2350:C:O2'   | 2.40                     | 0.54              |
| 24:X:58:ILE:HG12 | 24:X:66:VAL:HG21 | 1.88                     | 0.54              |
| 1:A:13:A:O2'     | 1:A:15:G:N7      | 2.39                     | 0.54              |
| 1:A:45:G:H5''    | 1:A:46:G:H5'     | 1.88                     | 0.54              |
| 1:A:2720:U:OP1   | 16:P:52:ARG:NH2  | 2.40                     | 0.54              |
| 1:A:358:U:H2'    | 1:A:359:G:H8     | 2.43                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1798:U:OP2   | 3:C:270:ARG:NH2   | 2.41                     | 0.54              |
| 3:C:70:LYS:HB3   | 3:C:73:ILE:HD12   | 1.90                     | 0.54              |
| 24:X:39:VAL:O    | 24:X:43:LYS:N     | 2.41                     | 0.54              |
| 1:A:1204:A:N6    | 1:A:1242:U:O4     | 2.41                     | 0.54              |
| 1:A:1309:G:H4'   | 29:2:7:PRO:HB2    | 1.90                     | 0.54              |
| 1:A:2229:U:H2'   | 1:A:2230:G:H8     | 1.72                     | 0.54              |
| 1:A:585:G:H21    | 1:A:1254:A:N6     | 2.06                     | 0.54              |
| 32:5:3:LEU:HD12  | 32:5:5:LEU:H      | 1.73                     | 0.54              |
| 1:A:550:C:H2'    | 1:A:551:G:H8      | 1.73                     | 0.54              |
| 1:A:713:G:H21    | 1:A:718:A:H62     | 1.55                     | 0.54              |
| 3:C:106:PRO:HD2  | 3:C:109:LEU:HD22  | 1.90                     | 0.54              |
| 1:A:538:A:N6     | 1:A:555:G:O2'     | 2.41                     | 0.54              |
| 2:B:48:U:OP2     | 15:O:30:ARG:NH2   | 2.41                     | 0.54              |
| 11:K:40:LYS:HE3  | 11:K:57:VAL:HG12  | 1.90                     | 0.54              |
| 3:C:165:ALA:HB3  | 3:C:172:THR:HB    | 1.90                     | 0.53              |
| 1:A:1800:C:N4    | 1:A:1818:U:O2'    | 2.42                     | 0.53              |
| 20:T:6:ARG:NH2   | 20:T:37:ASP:OD2   | 2.42                     | 0.53              |
| 1:A:589:U:H2'    | 1:A:590:A:H8      | 1.74                     | 0.53              |
| 1:A:1223:G:OP1   | 18:R:68:ARG:NH2   | 2.42                     | 0.53              |
| 1:A:1288:G:OP2   | 1:A:1288:G:N2     | 2.40                     | 0.53              |
| 1:A:2320:U:O2'   | 1:A:2322:A:N6     | 2.40                     | 0.53              |
| 32:5:22:ALA:HB3  | 32:5:87:GLU:HB2   | 1.89                     | 0.53              |
| 4:D:148:GLN:HB2  | 4:D:152:PRO:HG2   | 1.90                     | 0.53              |
| 7:G:8:VAL:HB     | 7:G:49:LEU:HB2    | 1.90                     | 0.53              |
| 11:K:43:ILE:HD12 | 11:K:56:ASP:HB2   | 1.91                     | 0.53              |
| 4:D:15:PHE:H     | 16:P:11:GLN:HE22  | 1.56                     | 0.53              |
| 1:A:2861:U:H2'   | 1:A:2862:G:H8     | 1.73                     | 0.53              |
| 1:A:745:G:C6     | 1:A:746:U:H6      | 2.26                     | 0.53              |
| 1:A:1818:U:H5'   | 3:C:156:SER:HB2   | 1.91                     | 0.53              |
| 1:A:958:U:OP2    | 13:M:14:LYS:NZ    | 2.41                     | 0.53              |
| 29:2:12:ARG:HE   | 29:2:44:VAL:HG21  | 1.74                     | 0.53              |
| 1:A:1270:C:H5''  | 1:A:1271:G:H5'    | 1.91                     | 0.53              |
| 1:A:537:G:H4'    | 10:J:5:THR:HG21   | 1.90                     | 0.53              |
| 14:N:44:LEU:HD23 | 14:N:113:ILE:HD13 | 1.90                     | 0.53              |
| 12:L:62:PRO:HD3  | 30:3:26:ALA:HB2   | 1.91                     | 0.53              |
| 1:A:523:C:O2     | 1:A:554:U:O2'     | 2.27                     | 0.53              |
| 13:M:75:GLU:HB3  | 13:M:90:GLU:HG3   | 1.90                     | 0.53              |
| 1:A:632:A:OP1    | 30:3:14:LYS:NZ    | 2.42                     | 0.52              |
| 1:A:1953:A:O2'   | 1:A:2559:C:O2     | 2.25                     | 0.52              |
| 11:K:30:ARG:NH2  | 11:K:37:ASP:OD2   | 2.41                     | 0.52              |
| 1:A:2394:C:H5''  | 12:L:63:LYS:HE3   | 1.91                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 20:T:38:ALA:HB1  | 20:T:43:ILE:HD11  | 1.91                     | 0.52              |
| 29:2:31:LEU:HG   | 29:2:42:LEU:HD21  | 1.90                     | 0.52              |
| 1:A:119:A:H4'    | 1:A:120:U:H5'     | 1.90                     | 0.52              |
| 6:F:152:ASP:N    | 6:F:152:ASP:OD1   | 2.42                     | 0.52              |
| 26:Z:10:ARG:HB2  | 26:Z:53:MET:HB2   | 1.90                     | 0.52              |
| 1:A:1796:U:H3    | 1:A:1823:G:H1     | 1.57                     | 0.52              |
| 1:A:576:U:H2'    | 1:A:577:G:C8      | 2.45                     | 0.52              |
| 12:L:109:LYS:HD2 | 12:L:126:ARG:HH11 | 1.74                     | 0.52              |
| 1:A:2659:G:N2    | 1:A:2662:A:OP2    | 2.42                     | 0.52              |
| 1:A:475:C:H4'    | 1:A:510:C:H5'     | 1.90                     | 0.52              |
| 11:K:9:ASN:OD1   | 11:K:18:ARG:NH1   | 2.43                     | 0.52              |
| 1:A:177:G:H3'    | 1:A:178:G:H8      | 1.73                     | 0.52              |
| 1:A:835:C:H2'    | 1:A:836:G:H8      | 1.73                     | 0.52              |
| 1:A:444:C:OP2    | 5:E:44:ARG:NH2    | 2.42                     | 0.52              |
| 1:A:2483:C:N3    | 13:M:123:LYS:NZ   | 2.58                     | 0.52              |
| 1:A:2693:G:H2'   | 1:A:2694:G:H8     | 1.75                     | 0.52              |
| 1:A:410:G:N3     | 1:A:432:A:N6      | 41.50                    | 0.52              |
| 1:A:877:A:O2'    | 1:A:900:A:N6      | 2.42                     | 0.52              |
| 10:J:17:VAL:HG23 | 10:J:137:PRO:HB2  | 1.91                     | 0.52              |
| 24:X:4:CYS:HB3   | 24:X:9:LYS:H      | 1.74                     | 0.52              |
| 1:A:1724:G:O6    | 1:A:1737:G:N2     | 2.43                     | 0.52              |
| 1:A:1753:G:H5''  | 16:P:92:ARG:HD3   | 1.90                     | 0.52              |
| 6:F:35:LEU:HB2   | 6:F:88:VAL:HB     | 1.91                     | 0.52              |
| 1:A:2307:G:H1    | 6:F:40:GLY:HA3    | 1.74                     | 0.52              |
| 10:J:56:VAL:HB   | 10:J:124:VAL:HG12 | 1.91                     | 0.52              |
| 1:A:2279:G:HO2'  | 1:A:2327:A:HO2'   | 1.56                     | 0.52              |
| 1:A:854:C:H2'    | 1:A:855:G:H8      | 1.75                     | 0.52              |
| 8:H:30:LEU:HB3   | 8:H:36:ALA:HB3    | 1.91                     | 0.52              |
| 8:H:47:PHE:HA    | 8:H:51:ARG:HB2    | 1.90                     | 0.52              |
| 1:A:2692:G:N3    | 1:A:2847:U:O2'    | 2.40                     | 0.52              |
| 1:A:727:A:OP2    | 1:A:1431:A:O2'    | 2.28                     | 0.52              |
| 4:D:131:ASP:O    | 4:D:136:ASN:ND2   | 2.41                     | 0.52              |
| 8:H:38:PRO:O     | 8:H:43:ASN:ND2    | 2.41                     | 0.52              |
| 18:R:35:PHE:O    | 18:R:58:VAL:HA    | 2.10                     | 0.52              |
| 29:2:34:ARG:NH2  | 29:2:41:ARG:O     | 2.43                     | 0.51              |
| 1:A:1013:C:H2'   | 1:A:1014:A:H8     | 1.74                     | 0.51              |
| 3:C:184:GLU:HG3  | 3:C:186:ASP:H     | 1.75                     | 0.51              |
| 1:A:1428:C:OP2   | 3:C:27:LYS:NZ     | 2.43                     | 0.51              |
| 1:A:1779:U:OP2   | 1:A:1784:A:N6     | 2.43                     | 0.51              |
| 1:A:2081:U:H2'   | 1:A:2082:A:H8     | 1.75                     | 0.51              |
| 1:A:227:A:H61    | 1:A:410:G:H21     | 1.58                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:2023:C:H2'   | 1:A:2024:G:H8    | 1.75                     | 0.51              |
| 1:A:407:G:H2'    | 1:A:408:G:H8     | 1.75                     | 0.51              |
| 1:A:1394:U:O2    | 20:T:19:LYS:NZ   | 2.41                     | 0.51              |
| 3:C:77:VAL:HG21  | 3:C:109:LEU:HD11 | 1.91                     | 0.51              |
| 13:M:35:ALA:O    | 13:M:99:GLY:N    | 2.42                     | 0.51              |
| 1:A:532:A:N6     | 1:A:1206:G:O2'   | 61.77                    | 0.51              |
| 1:A:674:G:H2'    | 1:A:675:A:H8     | 3.81                     | 0.51              |
| 1:A:767:U:H2'    | 1:A:768:G:H8     | 1.76                     | 0.51              |
| 1:A:787:C:H5''   | 1:A:788:A:H5'    | 1.92                     | 0.51              |
| 1:A:878:A:H3'    | 1:A:879:G:H8     | 1.75                     | 0.51              |
| 8:H:132:PHE:H    | 8:H:140:ALA:HB3  | 1.74                     | 0.51              |
| 8:H:1:MET:N      | 8:H:20:ASN:OD1   | 2.43                     | 0.51              |
| 15:O:108:ASP:OD1 | 15:O:111:ARG:NH1 | 2.43                     | 0.51              |
| 9:I:45:THR:HG22  | 9:I:50:LYS:HG2   | 1.93                     | 0.51              |
| 12:L:17:LYS:HE3  | 12:L:27:LEU:HD22 | 1.93                     | 0.51              |
| 31:4:19:ARG:HD2  | 31:4:24:ARG:HD2  | 1.92                     | 0.51              |
| 32:5:26:VAL:HG21 | 32:5:114:GLU:HG2 | 1.93                     | 0.51              |
| 1:A:297:G:N2     | 1:A:300:A:OP2    | 12.67                    | 0.51              |
| 32:5:56:ARG:HE   | 32:5:83:ALA:HB2  | 1.74                     | 0.50              |
| 32:5:68:PRO:HA   | 32:5:72:LEU:HG   | 1.93                     | 0.50              |
| 1:A:774:G:N2     | 1:A:787:C:O2'    | 2.44                     | 0.50              |
| 1:A:99:U:H5''    | 1:A:100:U:H5'    | 1.91                     | 0.50              |
| 27:0:27:LEU:HD23 | 27:0:36:LYS:HB3  | 1.94                     | 0.50              |
| 1:A:2110:G:N2    | 1:A:2179:C:N3    | 2.59                     | 0.50              |
| 11:K:12:ASP:HB3  | 11:K:99:ILE:HG12 | 1.94                     | 0.50              |
| 22:V:9:ARG:HD3   | 22:V:39:ALA:HB1  | 1.92                     | 0.50              |
| 1:A:1378:A:O2'   | 1:A:1380:G:OP2   | 2.30                     | 0.50              |
| 1:A:2008:C:H2'   | 1:A:2009:A:H8    | 1.75                     | 0.50              |
| 1:A:2539:C:H4'   | 31:4:36:ARG:HH12 | 1.77                     | 0.50              |
| 1:A:283:G:H1     | 1:A:357:C:H42    | 1.58                     | 0.50              |
| 1:A:481:G:O2'    | 1:A:506:G:N2     | 2.44                     | 0.50              |
| 1:A:672:C:OP2    | 12:L:42:SER:OG   | 2.29                     | 0.50              |
| 1:A:907:G:N2     | 13:M:70:ASP:OD2  | 2.44                     | 0.50              |
| 1:A:779:U:O2     | 1:A:785:G:O6     | 2.30                     | 0.50              |
| 4:D:55:LYS:HE2   | 4:D:77:ARG:HA    | 1.94                     | 0.50              |
| 10:J:36:LEU:HD22 | 10:J:121:LYS:HB2 | 1.92                     | 0.50              |
| 21:U:36:GLU:HA   | 21:U:61:GLU:HG2  | 1.93                     | 0.50              |
| 1:A:1326:U:H5'   | 1:A:2010:G:H21   | 1.77                     | 0.50              |
| 1:A:2360:G:H1'   | 12:L:60:ARG:HH22 | 1.77                     | 0.50              |
| 1:A:505:A:HO2'   | 1:A:509:C:HO2'   | 1.59                     | 0.50              |
| 1:A:848:C:H2'    | 1:A:849:A:H8     | 1.77                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:340:A:O2'    | 5:E:162:ARG:NH1  | 2.45                     | 0.50              |
| 1:A:1806:C:H1'   | 3:C:43:ASN:HD21  | 1.76                     | 0.50              |
| 1:A:2746:U:H5''  | 7:G:137:LYS:HE2  | 1.94                     | 0.50              |
| 6:F:163:GLU:OE1  | 6:F:166:ARG:NH1  | 2.45                     | 0.50              |
| 1:A:2295:C:OP1   | 15:O:10:ARG:NH1  | 2.44                     | 0.50              |
| 1:A:1068:G:N2    | 1:A:1095:A:O2'   | 2.36                     | 0.49              |
| 1:A:48:G:N2      | 1:A:177:G:OP2    | 2.44                     | 0.49              |
| 1:A:242:G:N2     | 1:A:255:A:OP2    | 2.42                     | 0.49              |
| 1:A:537:G:H22    | 1:A:555:G:H2'    | 1.77                     | 0.49              |
| 14:N:28:LEU:HD13 | 14:N:34:ILE:HG12 | 1.94                     | 0.49              |
| 1:A:464:U:H4'    | 29:2:12:ARG:HH22 | 1.76                     | 0.49              |
| 16:P:105:LYS:O   | 16:P:108:ARG:NH2 | 2.45                     | 0.49              |
| 25:Y:49:ASP:OD1  | 25:Y:52:ARG:NH2  | 2.45                     | 0.49              |
| 1:A:1754:A:N1    | 1:A:2716:C:O2'   | 2.44                     | 0.49              |
| 1:A:1899:A:H4'   | 1:A:1901:A:H5''  | 1.93                     | 0.49              |
| 1:A:76:C:OP1     | 25:Y:48:ARG:NH1  | 2.46                     | 0.49              |
| 1:A:1080:A:H1'   | 9:I:127:SER:HA   | 1.94                     | 0.49              |
| 1:A:1807:G:N2    | 1:A:1810:A:OP2   | 2.44                     | 0.49              |
| 1:A:574:A:N6     | 1:A:2034:U:OP1   | 2.43                     | 0.49              |
| 1:A:2788:C:O2'   | 1:A:2809:A:N3    | 2.41                     | 0.49              |
| 1:A:966:G:H4'    | 1:A:2271:G:H22   | 1.78                     | 0.49              |
| 11:K:87:LEU:HD13 | 11:K:92:GLU:HB3  | 1.94                     | 0.49              |
| 1:A:1682:G:OP2   | 1:A:1699:G:N2    | 2.44                     | 0.49              |
| 1:A:1111:A:HO2'  | 7:G:2:ARG:HH22   | 1.58                     | 0.49              |
| 31:4:36:ARG:HD3  | 31:4:37:GLN:H    | 1.78                     | 0.49              |
| 1:A:2291:U:O2'   | 1:A:2374:C:O2    | 2.31                     | 0.49              |
| 1:A:2002:G:OP2   | 14:N:9:GLN:NE2   | 2.46                     | 0.49              |
| 1:A:746:U:H1'    | 1:A:748:G:N2     | 2.28                     | 0.49              |
| 1:A:1022:G:N2    | 1:A:1023:U:O4    | 2.45                     | 0.49              |
| 1:A:1049:C:H2'   | 1:A:1050:A:H8    | 1.78                     | 0.49              |
| 1:A:2258:C:O2'   | 1:A:2427:C:OP2   | 2.31                     | 0.49              |
| 1:A:598:U:H2'    | 1:A:599:A:H8     | 1.78                     | 0.49              |
| 3:C:1:ALA:N      | 3:C:19:VAL:O     | 2.43                     | 0.49              |
| 1:A:2060:A:H62   | 5:E:69:ARG:HH22  | 1.60                     | 0.49              |
| 19:S:73:LYS:HB2  | 19:S:106:VAL:HB  | 1.94                     | 0.49              |
| 21:U:14:THR:OG1  | 21:U:68:ASN:ND2  | 2.44                     | 0.49              |
| 30:3:32:LEU:HB3  | 30:3:40:LYS:HD3  | 1.95                     | 0.49              |
| 33:7:25:A:C5     | 33:7:26:U:C5     | 3.01                     | 0.49              |
| 1:A:1024:G:O2'   | 1:A:1144:A:O2'   | 2.31                     | 0.49              |
| 12:L:20:GLY:H    | 12:L:28:GLY:HA2  | 1.77                     | 0.49              |
| 1:A:1173:U:O2'   | 1:A:1177:G:N2    | 2.40                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:2113:U:O4    | 1:A:2119:A:N6    | 2.45                     | 0.48              |
| 1:A:28:A:O2'     | 1:A:296:U:OP1    | 49.04                    | 0.48              |
| 1:A:629:G:H1'    | 1:A:639:U:H1'    | 1.95                     | 0.48              |
| 1:A:737:C:N4     | 1:A:738:G:O6     | 2.46                     | 0.48              |
| 2:B:5:U:OP1      | 2:B:61:G:O2'     | 2.29                     | 0.48              |
| 3:C:243:PRO:O    | 3:C:250:GLN:NE2  | 2.46                     | 0.48              |
| 2:B:95:U:H2'     | 2:B:96:G:H8      | 1.79                     | 0.48              |
| 3:C:140:VAL:HG12 | 3:C:191:LEU:HD23 | 1.93                     | 0.48              |
| 31:4:3:VAL:HA    | 31:4:36:ARG:HB3  | 1.94                     | 0.48              |
| 8:H:94:ILE:HG23  | 8:H:98:ASP:HB2   | 1.95                     | 0.48              |
| 1:A:2647:U:H2'   | 1:A:2648:G:H8    | 1.78                     | 0.48              |
| 1:A:466:A:OP1    | 29:2:34:ARG:NH1  | 2.46                     | 0.48              |
| 5:E:75:SER:HB3   | 5:E:78:TRP:HD1   | 1.77                     | 0.48              |
| 9:I:44:LYS:HG2   | 9:I:70:THR:HG21  | 1.95                     | 0.48              |
| 1:A:1469:A:OP2   | 1:A:1522:A:N6    | 2.47                     | 0.48              |
| 1:A:177:G:N2     | 1:A:177:G:OP2    | 2.36                     | 0.48              |
| 1:A:2345:G:H4'   | 1:A:2346:A:H3'   | 1.95                     | 0.48              |
| 5:E:97:ASN:ND2   | 5:E:100:MET:SD   | 2.86                     | 0.48              |
| 1:A:2233:U:H2'   | 1:A:2234:G:H8    | 1.77                     | 0.48              |
| 1:A:2822:G:O2'   | 1:A:2825:G:N1    | 2.40                     | 0.48              |
| 2:B:1:U:H2'      | 2:B:2:G:H8       | 1.78                     | 0.48              |
| 8:H:17:ASP:HB3   | 8:H:19:VAL:HG23  | 1.96                     | 0.48              |
| 1:A:631:A:N3     | 1:A:2415:G:O2'   | 2.40                     | 0.48              |
| 4:D:36:GLN:OE1   | 4:D:49:GLN:NE2   | 2.46                     | 0.48              |
| 1:A:673:C:OP1    | 5:E:49:ARG:NH2   | 2.45                     | 0.48              |
| 1:A:807:U:O2'    | 1:A:2060:A:N1    | 2.42                     | 0.48              |
| 1:A:2076:U:OP2   | 1:A:2238:G:N2    | 2.45                     | 0.48              |
| 1:A:2618:G:H21   | 4:D:155:VAL:HG21 | 1.78                     | 0.48              |
| 1:A:451:U:O2     | 1:A:453:A:N6     | 2.47                     | 0.48              |
| 1:A:1129:A:O2'   | 1:A:2515:C:O2    | 2.29                     | 0.47              |
| 1:A:291:G:H1     | 1:A:349:U:H3     | 1.61                     | 0.47              |
| 9:I:102:ARG:NH1  | 9:I:106:GLN:OE1  | 2.47                     | 0.47              |
| 1:A:1830:C:H2'   | 1:A:1831:G:H8    | 1.79                     | 0.47              |
| 1:A:2848:G:O2'   | 1:A:2868:A:N6    | 2.46                     | 0.47              |
| 1:A:776:G:H22    | 1:A:2072:C:H5'   | 1.80                     | 0.47              |
| 1:A:776:G:N2     | 1:A:802:A:OP2    | 24.26                    | 0.47              |
| 5:E:182:ALA:HB2  | 12:L:3:LEU:HD22  | 1.96                     | 0.47              |
| 17:Q:87:VAL:HG13 | 18:R:49:ILE:HD11 | 1.96                     | 0.47              |
| 1:A:1323:C:OP1   | 19:S:98:LYS:NZ   | 2.45                     | 0.47              |
| 1:A:1638:C:O2    | 1:A:2698:U:O2'   | 2.32                     | 0.47              |
| 1:A:659:G:O2'    | 5:E:95:LYS:O     | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:28:GLY:H    | 12:L:31:GLY:HA2  | 1.78                     | 0.47              |
| 16:P:25:VAL:HG22 | 16:P:85:VAL:HG22 | 1.96                     | 0.47              |
| 1:A:1069:A:N7    | 1:A:1073:A:N6    | 2.62                     | 0.47              |
| 1:A:335:C:O2'    | 1:A:1433:A:N3    | 112.66                   | 0.47              |
| 1:A:1936:A:OP2   | 1:A:1962:C:N4    | 2.41                     | 0.47              |
| 1:A:213:A:H2'    | 1:A:214:G:C8     | 2.50                     | 0.47              |
| 6:F:9:ASP:OD1    | 6:F:9:ASP:N      | 2.45                     | 0.47              |
| 21:U:20:LYS:HB3  | 21:U:38:ILE:HD12 | 1.96                     | 0.47              |
| 1:A:720:U:H2'    | 1:A:721:A:H8     | 1.80                     | 0.47              |
| 1:A:1429:G:H2'   | 1:A:1430:G:H8    | 1.79                     | 0.47              |
| 1:A:302:C:H2'    | 1:A:303:G:H8     | 1.79                     | 0.47              |
| 2:B:7:G:O2'      | 15:O:38:GLN:NE2  | 2.47                     | 0.47              |
| 20:T:13:ALA:HB3  | 20:T:33:LYS:HD3  | 1.96                     | 0.47              |
| 14:N:118:ARG:NH1 | 27:O:55:ALA:O    | 2.48                     | 0.47              |
| 31:4:30:GLU:HG3  | 31:4:32:LYS:H    | 1.80                     | 0.47              |
| 1:A:1046:A:H4'   | 32:5:61:ARG:HB3  | 1.95                     | 0.47              |
| 1:A:1071:G:N2    | 1:A:1089:A:O2'   | 2.45                     | 0.47              |
| 1:A:1432:G:O5'   | 16:P:105:LYS:HG2 | 54.57                    | 0.47              |
| 1:A:806:C:O2     | 1:A:2444:G:O2'   | 2.33                     | 0.47              |
| 1:A:917:A:H5''   | 1:A:2268:A:H61   | 1.80                     | 0.47              |
| 22:V:77:VAL:HG23 | 22:V:89:ILE:HG12 | 1.95                     | 0.47              |
| 26:Z:16:LEU:HB2  | 26:Z:19:HIS:HD2  | 1.79                     | 0.47              |
| 1:A:290:U:H2'    | 1:A:291:G:H8     | 1.80                     | 0.47              |
| 1:A:239:C:HO2'   | 1:A:622:G:HO2'   | 1.61                     | 0.47              |
| 11:K:35:VAL:HG11 | 11:K:106:GLU:HB2 | 1.97                     | 0.47              |
| 14:N:43:GLU:OE2  | 14:N:46:ARG:NH2  | 2.47                     | 0.47              |
| 1:A:1597:A:H4'   | 1:A:1598:A:H8    | 1.80                     | 0.47              |
| 1:A:2512:C:OP2   | 4:D:128:ARG:NH2  | 2.48                     | 0.47              |
| 1:A:376:G:H2'    | 1:A:377:G:H8     | 2.07                     | 0.47              |
| 33:7:26:U:H2'    | 33:7:27:G:C1'    | 2.45                     | 0.47              |
| 1:A:2458:G:O2'   | 1:A:2460:U:O4    | 2.32                     | 0.47              |
| 1:A:2768:U:O2'   | 10:J:95:ARG:NH2  | 2.48                     | 0.47              |
| 1:A:590:A:H61    | 1:A:667:U:H3     | 1.62                     | 0.47              |
| 6:F:55:ASP:OD2   | 6:F:149:ARG:NH2  | 2.47                     | 0.47              |
| 13:M:40:ARG:HH11 | 13:M:93:VAL:HG11 | 1.79                     | 0.47              |
| 20:T:37:ASP:OD1  | 20:T:37:ASP:N    | 2.47                     | 0.47              |
| 1:A:320:A:HO2'   | 1:A:1435:G:HO2'  | 124.49                   | 0.47              |
| 1:A:651:G:H5'    | 30:3:18:LYS:HG3  | 1.98                     | 0.46              |
| 2:B:114:C:H2'    | 2:B:115:A:H8     | 1.79                     | 0.46              |
| 3:C:267:VAL:HG12 | 3:C:268:ARG:HG2  | 1.97                     | 0.46              |
| 12:L:62:PRO:HG2  | 30:3:24:LYS:HB3  | 1.96                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1209:U:H4'    | 1:A:1212:G:H4'    | 1.97                     | 0.46              |
| 1:A:577:G:O2'     | 1:A:1254:A:OP1    | 2.32                     | 0.46              |
| 1:A:1333:G:H2'    | 1:A:1334:G:H8     | 1.81                     | 0.46              |
| 1:A:582:A:H2'     | 1:A:583:G:H8      | 1.81                     | 0.46              |
| 1:A:690:G:H4'     | 3:C:216:ARG:HH22  | 1.80                     | 0.46              |
| 22:V:20:LEU:HD11  | 22:V:41:GLU:HG3   | 1.97                     | 0.46              |
| 29:2:31:LEU:HD23  | 29:2:35:ARG:HH12  | 1.80                     | 0.46              |
| 32:5:24:SER:HB2   | 32:5:116:GLU:HG3  | 1.97                     | 0.46              |
| 1:A:633:A:O2'     | 1:A:2404:U:OP1    | 2.33                     | 0.46              |
| 1:A:377:G:H1      | 1:A:397:U:H3      | 1.63                     | 0.46              |
| 19:S:69:LEU:HA    | 19:S:109:ASP:HA   | 1.97                     | 0.46              |
| 1:A:519:U:H2'     | 1:A:520:G:H8      | 1.80                     | 0.46              |
| 3:C:141:HIS:ND1   | 3:C:192:GLY:O     | 2.43                     | 0.46              |
| 5:E:3:LEU:HD13    | 5:E:120:VAL:HG21  | 1.97                     | 0.46              |
| 1:A:1432:G:H2'    | 1:A:1433:A:H8     | 1.81                     | 0.46              |
| 1:A:1291:C:H2'    | 1:A:1292:G:H8     | 1.81                     | 0.46              |
| 1:A:1447:C:O2'    | 1:A:1544:A:N3     | 2.39                     | 0.46              |
| 1:A:2523:G:O2'    | 1:A:2764:A:O2'    | 2.31                     | 0.46              |
| 1:A:476:G:O2'     | 1:A:502:A:N6      | 2.45                     | 0.46              |
| 10:J:36:LEU:HD11  | 10:J:122:LEU:HD13 | 1.97                     | 0.46              |
| 18:R:1:MET:N      | 18:R:42:ALA:O     | 2.36                     | 0.46              |
| 32:5:33:VAL:HG12  | 32:5:35:VAL:H     | 1.80                     | 0.46              |
| 1:A:1921:G:H2'    | 1:A:1922:G:H8     | 1.80                     | 0.46              |
| 1:A:2245:U:H5''   | 1:A:2246:G:H5'    | 1.96                     | 0.46              |
| 1:A:254:G:OP2     | 30:3:4:LYS:NZ     | 2.45                     | 0.46              |
| 1:A:720:U:H2'     | 1:A:721:A:C8      | 2.51                     | 0.46              |
| 6:F:115:GLY:HA3   | 6:F:177:ARG:HB2   | 1.97                     | 0.46              |
| 12:L:127:VAL:HG21 | 12:L:142:ILE:HD13 | 1.97                     | 0.46              |
| 1:A:1368:G:H2'    | 1:A:1369:G:H8     | 1.81                     | 0.46              |
| 1:A:1387:A:H5'    | 1:A:1469:A:H1'    | 1.97                     | 0.46              |
| 1:A:1432:G:H2'    | 1:A:1433:A:C8     | 2.51                     | 0.46              |
| 1:A:568:U:O4      | 18:R:81:LYS:NZ    | 2.42                     | 0.46              |
| 1:A:196:A:H61     | 1:A:831:G:H21     | 1.64                     | 0.46              |
| 28:1:5:ARG:HG2    | 28:1:23:THR:HB    | 1.98                     | 0.46              |
| 33:7:25:A:C6      | 33:7:26:U:C4      | 3.03                     | 0.46              |
| 1:A:1386:C:H2'    | 1:A:1387:A:C8     | 2.51                     | 0.46              |
| 1:A:581:C:H2'     | 1:A:582:A:C8      | 2.51                     | 0.46              |
| 2:B:111:U:H2'     | 2:B:112:G:H8      | 1.81                     | 0.46              |
| 3:C:154:ALA:HB2   | 3:C:161:VAL:HG23  | 1.98                     | 0.46              |
| 1:A:2417:C:H5''   | 30:3:44:ARG:HG3   | 1.97                     | 0.45              |
| 1:A:212:G:H2'     | 1:A:213:A:C8      | 2.50                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:372:G:O6     | 24:X:56:ARG:NH2   | 2.49                     | 0.45              |
| 1:A:2052:A:O2'   | 4:D:149:ASN:O     | 2.35                     | 0.45              |
| 24:X:6:VAL:HA    | 24:X:73:ARG:HH22  | 1.79                     | 0.45              |
| 30:3:28:LEU:HA   | 30:3:32:LEU:HD11  | 1.98                     | 0.45              |
| 1:A:224:U:OP2    | 1:A:408:G:N2      | 2.41                     | 0.45              |
| 1:A:2313:C:H2'   | 1:A:2314:A:H8     | 1.79                     | 0.45              |
| 1:A:33:C:O2      | 1:A:447:A:N6      | 2.49                     | 0.45              |
| 1:A:351:C:H2'    | 1:A:352:A:H8      | 1.81                     | 0.45              |
| 1:A:373:U:H2'    | 1:A:374:A:H8      | 1.81                     | 0.45              |
| 8:H:70:GLU:HB2   | 8:H:134:VAL:HG21  | 1.98                     | 0.45              |
| 6:F:140:ILE:HG22 | 6:F:142:TYR:H     | 1.82                     | 0.45              |
| 5:E:102:ARG:NH1  | 5:E:200:LEU:O     | 2.49                     | 0.45              |
| 1:A:2348:U:OP2   | 30:3:41:ARG:NH1   | 2.50                     | 0.45              |
| 1:A:1254:A:H5''  | 1:A:1255:U:H5''   | 1.99                     | 0.45              |
| 1:A:2047:C:H2'   | 1:A:2048:G:H8     | 1.82                     | 0.45              |
| 1:A:2086:U:H2'   | 1:A:2087:G:C8     | 2.52                     | 0.45              |
| 1:A:2468:A:OP2   | 1:A:2476:A:N6     | 2.50                     | 0.45              |
| 10:J:32:LEU:HD22 | 10:J:54:ILE:HG21  | 1.99                     | 0.45              |
| 1:A:111:A:O2'    | 25:Y:58:ASN:ND2   | 2.50                     | 0.45              |
| 1:A:1997:C:H2'   | 1:A:1998:A:H8     | 1.82                     | 0.45              |
| 1:A:662:G:H2'    | 1:A:663:G:H8      | 1.80                     | 0.45              |
| 1:A:91:A:O2'     | 1:A:92:U:O4'      | 2.32                     | 0.45              |
| 4:D:115:GLY:HA2  | 4:D:166:GLY:HA3   | 1.98                     | 0.45              |
| 1:A:585:G:N2     | 1:A:1254:A:H62    | 2.14                     | 0.45              |
| 4:D:109:VAL:HG22 | 4:D:203:VAL:HG22  | 1.99                     | 0.45              |
| 10:J:31:GLU:HG2  | 10:J:142:ILE:HG12 | 1.98                     | 0.45              |
| 1:A:2293:G:OP1   | 15:O:94:ARG:NH1   | 2.50                     | 0.45              |
| 16:P:91:VAL:HG21 | 16:P:96:LEU:HD11  | 1.99                     | 0.45              |
| 1:A:1171:G:N2    | 1:A:1179:G:N7     | 2.65                     | 0.45              |
| 1:A:1636:U:H2'   | 1:A:1637:A:H8     | 1.82                     | 0.45              |
| 1:A:460:A:H62    | 1:A:469:G:H21     | 1.64                     | 0.45              |
| 17:Q:99:VAL:O    | 17:Q:102:LYS:NZ   | 2.49                     | 0.45              |
| 18:R:76:LYS:HB2  | 18:R:85:LYS:HB3   | 1.99                     | 0.45              |
| 1:A:1612:C:O2'   | 29:2:5:PHE:O      | 2.35                     | 0.45              |
| 1:A:592:A:O2'    | 30:3:63:TYR:OH    | 2.35                     | 0.45              |
| 1:A:1509:A:H2'   | 1:A:1510:G:C8     | 2.52                     | 0.45              |
| 1:A:29:U:O2      | 1:A:1215:G:O2'    | 2.34                     | 0.45              |
| 1:A:302:C:H2'    | 1:A:303:G:C8      | 2.52                     | 0.45              |
| 1:A:589:U:H2'    | 1:A:590:A:C8      | 2.51                     | 0.45              |
| 4:D:37:VAL:HG22  | 4:D:48:ILE:HG22   | 1.99                     | 0.45              |
| 32:5:30:SER:HB3  | 32:5:109:LYS:HD2  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:286:U:H2'    | 1:A:287:G:H8     | 1.82                     | 0.45              |
| 14:N:118:ARG:NH2 | 27:O:54:ILE:O    | 2.50                     | 0.44              |
| 1:A:1081:U:H5'   | 9:I:126:ARG:HH21 | 1.82                     | 0.44              |
| 1:A:2086:U:H2'   | 1:A:2087:G:H8    | 1.81                     | 0.44              |
| 1:A:2719:G:H4'   | 1:A:2846:G:H4'   | 1.98                     | 0.44              |
| 1:A:2818:U:H2'   | 1:A:2819:G:C8    | 2.52                     | 0.44              |
| 1:A:581:C:H2'    | 1:A:582:A:H8     | 1.81                     | 0.44              |
| 1:A:692:C:H5''   | 3:C:38:LYS:HB3   | 1.99                     | 0.44              |
| 1:A:2070:A:H2'   | 1:A:2071:A:H8    | 1.81                     | 0.44              |
| 1:A:2370:G:O2'   | 28:1:43:ARG:NH1  | 2.51                     | 0.44              |
| 1:A:764:A:N3     | 3:C:211:ARG:NH1  | 2.65                     | 0.44              |
| 3:C:130:PRO:HA   | 3:C:188:ARG:HA   | 2.00                     | 0.44              |
| 15:O:8:ILE:O     | 15:O:12:THR:OG1  | 2.29                     | 0.44              |
| 20:T:54:GLU:HB3  | 20:T:88:LYS:HD2  | 1.98                     | 0.44              |
| 25:Y:37:LEU:HD11 | 25:Y:42:LEU:HD12 | 1.98                     | 0.44              |
| 1:A:16:C:H2'     | 1:A:17:G:H8      | 1.81                     | 0.44              |
| 1:A:526:A:O2'    | 1:A:2043:C:O2    | 2.28                     | 0.44              |
| 1:A:2144:G:H1'   | 1:A:2147:A:H61   | 1.82                     | 0.44              |
| 1:A:2656:U:C2    | 1:A:2665:A:N7    | 2.85                     | 0.44              |
| 1:A:2771:C:O2'   | 4:D:173:GLN:NE2  | 2.47                     | 0.44              |
| 3:C:5:CYS:SG     | 3:C:12:ARG:NH2   | 2.91                     | 0.44              |
| 17:Q:93:ILE:HG23 | 18:R:13:ARG:HB2  | 1.99                     | 0.44              |
| 2:B:93:C:H2'     | 2:B:94:A:H8      | 1.82                     | 0.44              |
| 32:5:48:ALA:HB3  | 32:5:51:TYR:HE1  | 1.82                     | 0.44              |
| 1:A:2443:C:H2'   | 1:A:2444:G:C8    | 2.52                     | 0.44              |
| 1:A:2676:C:O2    | 1:A:2732:G:N2    | 2.47                     | 0.44              |
| 27:O:42:ILE:HG22 | 27:O:48:TYR:HB2  | 1.99                     | 0.44              |
| 1:A:1432:G:P     | 16:P:105:LYS:HG2 | 54.88                    | 0.44              |
| 1:A:2559:C:H2'   | 1:A:2560:A:H8    | 1.82                     | 0.44              |
| 1:A:552:U:H2'    | 1:A:553:G:H8     | 1.82                     | 0.44              |
| 1:A:6:A:N3       | 10:J:135:GLN:NE2 | 2.65                     | 0.44              |
| 19:S:17:VAL:HG12 | 19:S:76:VAL:HG21 | 2.00                     | 0.44              |
| 1:A:18:U:O2'     | 1:A:554:U:OP1    | 2.35                     | 0.44              |
| 6:F:28:PRO:HB2   | 6:F:168:LEU:HD22 | 2.00                     | 0.44              |
| 24:X:39:VAL:O    | 24:X:43:LYS:CA   | 2.65                     | 0.44              |
| 1:A:2776:A:O2'   | 1:A:2782:G:N7    | 2.46                     | 0.44              |
| 1:A:793:A:OP2    | 1:A:2071:A:O2'   | 2.28                     | 0.44              |
| 1:A:1796:U:H2'   | 1:A:1797:G:C8    | 2.53                     | 0.44              |
| 1:A:2899:A:H2'   | 1:A:2900:A:C8    | 2.53                     | 0.44              |
| 3:C:56:GLY:HA2   | 3:C:212:TRP:HA   | 2.00                     | 0.44              |
| 4:D:9:VAL:HA     | 4:D:197:THR:HG23 | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:56:LEU:HD13  | 6:F:88:VAL:HG23  | 2.00                     | 0.44              |
| 19:S:62:ASP:OD1  | 19:S:62:ASP:N    | 2.49                     | 0.44              |
| 1:A:198:C:H4'    | 1:A:2243:U:H4'   | 2.00                     | 0.43              |
| 1:A:2291:U:O2    | 1:A:2374:C:O2'   | 2.32                     | 0.43              |
| 1:A:1841:U:H2'   | 1:A:1842:G:H8    | 1.83                     | 0.43              |
| 1:A:2459:A:H2    | 13:M:78:LEU:HD21 | 1.83                     | 0.43              |
| 1:A:918:A:N3     | 2:B:80:U:O2'     | 2.42                     | 0.43              |
| 3:C:74:PRO:HB3   | 3:C:114:GLN:HE21 | 1.83                     | 0.43              |
| 6:F:42:ALA:HB3   | 6:F:84:ILE:HD12  | 2.00                     | 0.43              |
| 8:H:125:THR:HG23 | 8:H:146:VAL:HG12 | 1.99                     | 0.43              |
| 1:A:1266:G:N2    | 1:A:1269:A:OP2   | 13.21                    | 0.43              |
| 1:A:2035:G:H5''  | 1:A:2036:C:H5    | 1.83                     | 0.43              |
| 1:A:2691:C:H2'   | 1:A:2692:G:H8    | 1.82                     | 0.43              |
| 1:A:2898:U:H2'   | 1:A:2899:A:C8    | 2.54                     | 0.43              |
| 1:A:605:G:O2'    | 1:A:657:U:O2     | 2.33                     | 0.43              |
| 15:O:4:LYS:HE2   | 15:O:8:ILE:HD11  | 2.00                     | 0.43              |
| 1:A:2457:U:C5    | 1:A:2494:G:N1    | 2.62                     | 0.43              |
| 1:A:674:G:H2'    | 1:A:675:A:C8     | 4.24                     | 0.43              |
| 1:A:854:C:H2'    | 1:A:855:G:C8     | 2.53                     | 0.43              |
| 32:5:119:PRO:HG2 | 32:5:121:SER:HB2 | 2.01                     | 0.43              |
| 1:A:2246:G:H2'   | 1:A:2247:A:H8    | 1.84                     | 0.43              |
| 16:P:84:SER:OG   | 16:P:86:LYS:NZ   | 2.51                     | 0.43              |
| 16:P:88:ARG:HB3  | 16:P:112:ARG:HD3 | 2.01                     | 0.43              |
| 1:A:1093:G:N2    | 1:A:1098:A:H62   | 2.15                     | 0.43              |
| 1:A:1287:A:H62   | 14:N:106:ASP:HB3 | 1.83                     | 0.43              |
| 24:X:39:VAL:O    | 24:X:43:LYS:HA   | 2.19                     | 0.43              |
| 25:Y:24:GLU:HB3  | 25:Y:46:VAL:HG21 | 1.99                     | 0.43              |
| 8:H:30:LEU:HA    | 8:H:35:LYS:HB2   | 2.00                     | 0.43              |
| 11:K:76:VAL:H    | 16:P:72:VAL:HG22 | 1.83                     | 0.43              |
| 1:A:1431:A:H2'   | 1:A:1432:G:H8    | 1.82                     | 0.43              |
| 5:E:18:THR:HA    | 5:E:106:LYS:HE3  | 2.01                     | 0.43              |
| 19:S:77:ASP:N    | 19:S:77:ASP:OD1  | 2.52                     | 0.43              |
| 1:A:655:A:H4'    | 1:A:656:G:H5'    | 2.00                     | 0.43              |
| 5:E:145:ASP:HA   | 5:E:166:LYS:HB3  | 2.01                     | 0.43              |
| 5:E:75:SER:HB3   | 5:E:78:TRP:CD1   | 2.54                     | 0.43              |
| 1:A:2372:U:H2'   | 1:A:2373:G:H8    | 1.84                     | 0.43              |
| 19:S:22:ASP:OD1  | 19:S:25:ARG:NH2  | 2.51                     | 0.43              |
| 1:A:1295:C:H2'   | 1:A:1296:G:H8    | 1.84                     | 0.42              |
| 1:A:2175:C:H2'   | 1:A:2176:A:H8    | 1.84                     | 0.42              |
| 1:A:546:U:H2'    | 1:A:547:A:H4'    | 1.99                     | 0.42              |
| 1:A:2395:C:H2'   | 1:A:2396:G:H8    | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:239:C:O2'    | 1:A:622:G:O2'    | 2.33                     | 0.42              |
| 1:A:1024:G:HO2'  | 1:A:1144:A:HO2'  | 1.61                     | 0.42              |
| 1:A:1687:G:N2    | 1:A:1701:A:H62   | 2.16                     | 0.42              |
| 1:A:490:C:H2'    | 1:A:491:G:H8     | 8.71                     | 0.42              |
| 13:M:42:THR:HG22 | 13:M:93:VAL:HG12 | 2.01                     | 0.42              |
| 14:N:79:LEU:HD23 | 14:N:83:LEU:HD12 | 2.02                     | 0.42              |
| 1:A:2832:U:H1'   | 1:A:2834:G:C2    | 2.54                     | 0.42              |
| 3:C:121:ALA:HB1  | 3:C:127:ASN:HB3  | 2.02                     | 0.42              |
| 3:C:206:LYS:HE2  | 3:C:208:GLY:HA3  | 2.01                     | 0.42              |
| 1:A:2691:C:H2'   | 1:A:2692:G:C8    | 2.54                     | 0.42              |
| 9:I:56:VAL:HG22  | 9:I:68:PHE:HB2   | 2.00                     | 0.42              |
| 30:3:32:LEU:HD22 | 30:3:40:LYS:HG2  | 2.00                     | 0.42              |
| 1:A:818:G:N2     | 1:A:1189:A:H62   | 2.14                     | 0.42              |
| 1:A:1700:A:H3'   | 1:A:1701:A:H8    | 1.85                     | 0.42              |
| 1:A:2630:G:H2'   | 1:A:2631:G:C8    | 2.55                     | 0.42              |
| 1:A:4:U:H2'      | 1:A:5:A:H8       | 1.85                     | 0.42              |
| 9:I:89:SER:HB3   | 9:I:135:MET:HA   | 2.00                     | 0.42              |
| 12:L:23:ILE:HD13 | 18:R:84:ARG:HH22 | 1.83                     | 0.42              |
| 1:A:1665:A:H2'   | 1:A:1666:G:H8    | 1.84                     | 0.42              |
| 1:A:244:A:N6     | 1:A:254:G:H21    | 2.05                     | 0.42              |
| 1:A:2006:C:O2'   | 1:A:2823:A:N3    | 2.51                     | 0.42              |
| 1:A:414:C:H2'    | 1:A:415:A:H8     | 1.84                     | 0.42              |
| 1:A:568:U:N3     | 1:A:571:U:OP2    | 2.46                     | 0.42              |
| 1:A:788:A:OP1    | 1:A:791:C:N4     | 2.42                     | 0.42              |
| 3:C:70:LYS:O     | 3:C:117:SER:OG   | 2.31                     | 0.42              |
| 5:E:47:LYS:HB2   | 5:E:51:GLU:HB2   | 2.01                     | 0.42              |
| 18:R:6:GLN:HE21  | 18:R:11:GLN:NE2  | 2.16                     | 0.42              |
| 21:U:28:LEU:HD12 | 21:U:32:LYS:HB2  | 2.00                     | 0.42              |
| 1:A:2313:C:H2'   | 1:A:2314:A:C8    | 2.54                     | 0.42              |
| 1:A:2836:U:H2'   | 1:A:2837:A:H8    | 1.85                     | 0.42              |
| 1:A:849:A:H61    | 1:A:929:U:H3     | 1.68                     | 0.42              |
| 1:A:2279:G:O2'   | 1:A:2327:A:O2'   | 2.30                     | 0.42              |
| 1:A:2447:G:N2    | 1:A:2450:A:N7    | 2.67                     | 0.42              |
| 1:A:2497:A:H1'   | 1:A:2498:C:H5    | 1.85                     | 0.42              |
| 17:Q:88:GLU:O    | 18:R:11:GLN:NE2  | 2.53                     | 0.42              |
| 1:A:1251:C:O2'   | 1:A:1253:A:OP2   | 2.38                     | 0.42              |
| 1:A:2131:U:H5'   | 1:A:2132:U:H5''  | 2.01                     | 0.42              |
| 1:A:2240:U:H2'   | 1:A:2241:A:H8    | 1.84                     | 0.42              |
| 2:B:114:C:H2'    | 2:B:115:A:C8     | 2.54                     | 0.42              |
| 3:C:75:ALA:HB3   | 3:C:115:ILE:HG13 | 2.01                     | 0.42              |
| 1:A:1716:U:H2'   | 1:A:1717:A:H8    | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:2801:G:H2'   | 1:A:2802:G:H8    | 1.85                     | 0.41              |
| 2:B:44:G:H1'     | 2:B:47:C:H42     | 1.85                     | 0.41              |
| 13:M:66:ARG:NH1  | 13:M:104:GLU:OE2 | 2.52                     | 0.41              |
| 9:I:117:THR:HG22 | 32:5:42:ARG:HH21 | 1.85                     | 0.41              |
| 1:A:1431:A:H2'   | 1:A:1432:G:C8    | 2.55                     | 0.41              |
| 1:A:2327:A:H2'   | 1:A:2328:A:C8    | 2.55                     | 0.41              |
| 1:A:249:C:O2     | 30:3:11:LYS:NZ   | 2.47                     | 0.41              |
| 1:A:406:G:H2'    | 1:A:407:G:H8     | 1.84                     | 0.41              |
| 1:A:4:U:H2'      | 1:A:5:A:C8       | 2.55                     | 0.41              |
| 1:A:781:A:OP1    | 3:C:216:ARG:NH2  | 2.51                     | 0.41              |
| 3:C:38:LYS:HE3   | 3:C:59:GLN:HG2   | 2.02                     | 0.41              |
| 14:N:45:ARG:HG2  | 14:N:95:THR:HG21 | 2.02                     | 0.41              |
| 20:T:22:THR:HA   | 20:T:25:GLU:HG2  | 2.01                     | 0.41              |
| 1:A:1435:G:H2'   | 1:A:1436:G:C8    | 2.56                     | 0.41              |
| 1:A:151:C:H2'    | 1:A:152:A:H8     | 1.86                     | 0.41              |
| 1:A:1847:G:HO2'  | 1:A:1848:A:H8    | 1.68                     | 0.41              |
| 1:A:2821:A:OP2   | 4:D:115:GLY:N    | 2.51                     | 0.41              |
| 1:A:476:G:N1     | 1:A:479:A:OP2    | 2.40                     | 0.41              |
| 1:A:532:A:OP1    | 1:A:561:G:N2     | 2.43                     | 0.41              |
| 1:A:533:G:O5'    | 17:Q:27:ARG:NH1  | 2.54                     | 0.41              |
| 1:A:746:U:H1'    | 1:A:748:G:H21    | 1.85                     | 0.41              |
| 1:A:828:U:O4     | 1:A:858:G:N2     | 39.89                    | 0.41              |
| 1:A:1140:C:H5'   | 10:J:26:GLY:HA3  | 2.03                     | 0.41              |
| 1:A:693:A:O2'    | 1:A:1353:A:N3    | 2.53                     | 0.41              |
| 1:A:2023:C:H2'   | 1:A:2024:G:C8    | 2.55                     | 0.41              |
| 1:A:2581:G:N2    | 1:A:2581:G:OP2   | 2.37                     | 0.41              |
| 1:A:2781:A:H5''  | 1:A:2782:G:H5'   | 2.02                     | 0.41              |
| 1:A:5:A:H2'      | 1:A:6:A:C8       | 2.55                     | 0.41              |
| 20:T:8:LEU:HD11  | 25:Y:22:LEU:HD12 | 2.01                     | 0.41              |
| 1:A:2863:C:H2'   | 1:A:2864:G:H8    | 1.86                     | 0.41              |
| 1:A:742:A:H2'    | 1:A:743:A:C8     | 2.55                     | 0.41              |
| 6:F:91:ARG:HA    | 6:F:95:MET:HB3   | 2.03                     | 0.41              |
| 1:A:2140:G:H2'   | 1:A:2141:G:H8    | 1.85                     | 0.41              |
| 1:A:2215:C:H2'   | 1:A:2216:G:C8    | 2.56                     | 0.41              |
| 1:A:2329:U:H2'   | 1:A:2330:G:C8    | 2.55                     | 0.41              |
| 1:A:453:A:N3     | 1:A:457:A:O2'    | 2.51                     | 0.41              |
| 1:A:545:U:N3     | 1:A:548:G:N1     | 2.45                     | 0.41              |
| 1:A:1433:A:H2'   | 1:A:1434:A:C8    | 2.55                     | 0.41              |
| 1:A:1592:C:H2'   | 1:A:1593:A:H8    | 1.85                     | 0.41              |
| 1:A:1858:A:N6    | 1:A:1884:G:O2'   | 2.48                     | 0.41              |
| 1:A:2073:C:HO2'  | 1:A:2598:A:HO2'  | 1.68                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:410:G:N2      | 1:A:432:A:N7      | 41.25                    | 0.41              |
| 1:A:572:A:H61     | 1:A:2029:G:H21    | 1.69                     | 0.41              |
| 20:T:58:VAL:HG22  | 20:T:85:VAL:HG13  | 2.02                     | 0.41              |
| 22:V:72:VAL:HB    | 22:V:91:PHE:HB3   | 2.01                     | 0.41              |
| 23:W:61:GLY:CA    | 23:W:79:GLU:O     | 2.66                     | 0.41              |
| 1:A:1433:A:H2'    | 1:A:1434:A:H8     | 1.86                     | 0.41              |
| 1:A:1744:A:H3'    | 1:A:1745:A:H8     | 1.86                     | 0.41              |
| 1:A:2036:C:H2'    | 1:A:2037:A:C8     | 2.56                     | 0.41              |
| 9:I:53:PRO:HG2    | 9:I:77:VAL:HG11   | 2.02                     | 0.41              |
| 13:M:47:GLU:OE2   | 13:M:51:ARG:NE    | 2.54                     | 0.41              |
| 15:O:69:ASP:N     | 15:O:69:ASP:OD1   | 2.50                     | 0.41              |
| 27:O:39:ARG:O     | 27:O:41:HIS:ND1   | 2.54                     | 0.41              |
| 1:A:1939:U:H5''   | 1:A:2604:U:C5     | 2.56                     | 0.41              |
| 1:A:2110:G:N1     | 1:A:2120:G:N7     | 2.69                     | 0.41              |
| 1:A:2692:G:H2'    | 1:A:2693:G:C8     | 2.56                     | 0.41              |
| 1:A:521:U:H2'     | 1:A:522:A:H8      | 1.85                     | 0.41              |
| 1:A:728:G:H4'     | 3:C:12:ARG:HD3    | 2.02                     | 0.41              |
| 1:A:832:U:H2'     | 1:A:833:A:C8      | 2.55                     | 0.41              |
| 1:A:974:G:H1'     | 1:A:975:A:C8      | 2.56                     | 0.41              |
| 2:B:45:A:O4'      | 6:F:91:ARG:NH2    | 2.54                     | 0.41              |
| 7:G:23:ILE:HG21   | 7:G:71:LEU:HD21   | 2.03                     | 0.41              |
| 28:I:36:LYS:HG3   | 28:I:47:ILE:HG13  | 2.02                     | 0.41              |
| 1:A:112:U:H5'     | 25:Y:58:ASN:HD21  | 1.85                     | 0.41              |
| 1:A:1227:G:OP2    | 17:Q:15:LYS:NZ    | 2.50                     | 0.41              |
| 1:A:1355:G:H2'    | 1:A:1356:G:H8     | 1.98                     | 0.41              |
| 1:A:1372:U:O2'    | 1:A:2212:A:N3     | 2.48                     | 0.41              |
| 1:A:414:C:H2'     | 1:A:415:A:C8      | 2.56                     | 0.41              |
| 5:E:149:ILE:HD11  | 5:E:172:ALA:HA    | 2.03                     | 0.41              |
| 14:N:42:LYS:HA    | 14:N:45:ARG:HE    | 1.86                     | 0.41              |
| 16:P:29:VAL:HG22  | 16:P:80:VAL:HG12  | 2.01                     | 0.41              |
| 20:T:37:ASP:O     | 20:T:81:LYS:NZ    | 2.54                     | 0.41              |
| 1:A:1030:C:H2'    | 1:A:1031:G:C8     | 2.56                     | 0.41              |
| 1:A:1355:G:H2'    | 1:A:1356:G:C8     | 2.81                     | 0.41              |
| 1:A:1827:U:OP2    | 3:C:220:ARG:NH1   | 2.53                     | 0.41              |
| 1:A:318:C:H2'     | 1:A:319:G:C8      | 2.54                     | 0.41              |
| 1:A:690:G:H21     | 3:C:42:ARG:HH12   | 1.69                     | 0.41              |
| 1:A:953:G:H2'     | 1:A:954:G:H8      | 1.86                     | 0.41              |
| 1:A:994:C:OP1     | 17:Q:52:ARG:NH2   | 2.54                     | 0.41              |
| 2:B:14:U:OP2      | 2:B:70:C:O2'      | 2.38                     | 0.41              |
| 5:E:106:LYS:HG3   | 5:E:200:LEU:HD23  | 2.03                     | 0.41              |
| 11:K:103:VAL:HG21 | 11:K:116:ILE:HG22 | 2.03                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1158:C:H5'' | 26:Z:30:ARG:HD2  | 2.03                     | 0.41              |
| 1:A:1202:G:O6   | 1:A:1244:A:N6    | 2.53                     | 0.40              |
| 1:A:1313:U:H4'  | 1:A:1332:G:H4'   | 2.03                     | 0.40              |
| 1:A:225:C:N3    | 1:A:231:A:N6     | 2.69                     | 0.40              |
| 1:A:2632:A:H2'  | 1:A:2633:G:C8    | 2.56                     | 0.40              |
| 1:A:1662:U:O2'  | 1:A:2687:U:OP1   | 2.39                     | 0.40              |
| 1:A:480:A:OP2   | 21:U:43:LYS:NZ   | 2.43                     | 0.40              |
| 1:A:1745:A:H2'  | 1:A:1746:A:H8    | 1.86                     | 0.40              |
| 1:A:2863:C:H2'  | 1:A:2864:G:C8    | 2.56                     | 0.40              |
| 1:A:471:A:OP1   | 5:E:79:ARG:NH1   | 2.49                     | 0.40              |
| 1:A:523:C:H2'   | 1:A:524:G:C8     | 2.56                     | 0.40              |
| 1:A:576:U:H2'   | 1:A:577:G:H8     | 1.87                     | 0.40              |
| 2:B:78:A:N6     | 2:B:98:G:H21     | 2.14                     | 0.40              |
| 1:A:434:U:O2'   | 1:A:436:C:N4     | 2.55                     | 0.40              |
| 1:A:598:U:H2'   | 1:A:599:A:C8     | 2.56                     | 0.40              |
| 1:A:1787:A:OP1  | 3:C:237:ARG:NH2  | 2.55                     | 0.40              |
| 10:J:45:THR:HB  | 10:J:48:VAL:HB   | 2.03                     | 0.40              |
| 1:A:1675:C:O2   | 4:D:133:THR:OG1  | 2.37                     | 0.40              |
| 1:A:2250:G:O2'  | 1:A:2496:C:OP1   | 2.26                     | 0.40              |
| 1:A:341:C:H2'   | 1:A:342:A:C8     | 2.57                     | 0.40              |
| 8:H:113:SER:O   | 8:H:116:ARG:NH1  | 2.48                     | 0.40              |
| 11:K:21:CYS:HA  | 11:K:41:ILE:HG22 | 2.02                     | 0.40              |
| 12:L:96:LYS:HE3 | 12:L:103:ILE:HA  | 2.04                     | 0.40              |
| 1:A:910:A:H62   | 13:M:12:MET:HA   | 1.86                     | 0.40              |
| 1:A:1704:C:H2'  | 1:A:1705:A:C8    | 2.57                     | 0.40              |
| 1:A:2289:G:H2'  | 1:A:2290:G:H8    | 1.86                     | 0.40              |
| 1:A:305:C:H2'   | 1:A:306:U:C6     | 2.57                     | 0.40              |
| 1:A:881:G:H2'   | 1:A:882:G:C8     | 2.56                     | 0.40              |
| 4:D:47:ALA:HB2  | 4:D:83:ARG:HD2   | 2.02                     | 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 |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3   | C     | 269/271 (99%) | 261 (97%) | 8 (3%)   | 0        | 100         | 100 |
| 4   | D     | 207/209 (99%) | 194 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 5   | E     | 199/201 (99%) | 188 (94%) | 11 (6%)  | 0        | 100         | 100 |
| 6   | F     | 175/177 (99%) | 161 (92%) | 14 (8%)  | 0        | 100         | 100 |
| 7   | G     | 174/176 (99%) | 161 (92%) | 10 (6%)  | 3 (2%)   | 10          | 48  |
| 8   | H     | 147/149 (99%) | 138 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 9   | I     | 139/141 (99%) | 121 (87%) | 18 (13%) | 0        | 100         | 100 |
| 10  | J     | 140/142 (99%) | 137 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 11  | K     | 120/122 (98%) | 107 (89%) | 13 (11%) | 0        | 100         | 100 |
| 12  | L     | 141/143 (99%) | 124 (88%) | 16 (11%) | 1 (1%)   | 24          | 64  |
| 13  | M     | 134/136 (98%) | 124 (92%) | 8 (6%)   | 2 (2%)   | 11          | 51  |
| 14  | N     | 118/120 (98%) | 110 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 15  | O     | 114/116 (98%) | 109 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 16  | P     | 112/114 (98%) | 105 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 17  | Q     | 115/117 (98%) | 113 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 18  | R     | 101/103 (98%) | 94 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 19  | S     | 108/110 (98%) | 100 (93%) | 7 (6%)   | 1 (1%)   | 19          | 59  |
| 20  | T     | 91/93 (98%)   | 82 (90%)  | 9 (10%)  | 0        | 100         | 100 |
| 21  | U     | 100/102 (98%) | 89 (89%)  | 10 (10%) | 1 (1%)   | 17          | 57  |
| 22  | V     | 92/94 (98%)   | 91 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 23  | W     | 73/75 (97%)   | 69 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 24  | X     | 75/77 (97%)   | 72 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 25  | Y     | 61/63 (97%)   | 59 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 26  | Z     | 56/58 (97%)   | 55 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 27  | 0     | 54/56 (96%)   | 53 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 28  | 1     | 48/50 (96%)   | 46 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 29  | 2     | 44/46 (96%)   | 43 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 30  | 3     | 62/64 (97%)   | 56 (90%)  | 4 (6%)   | 2 (3%)   | 4           | 36  |
| 31  | 4     | 36/38 (95%)   | 31 (86%)  | 5 (14%)  | 0        | 100         | 100 |
| 32  | 5     | 129/131 (98%) | 102 (79%) | 27 (21%) | 0        | 100         | 100 |
| 35  | b     | 216/218 (99%) | 196 (91%) | 19 (9%)  | 1 (0%)   | 31          | 71  |
| 36  | c     | 204/206 (99%) | 196 (96%) | 6 (3%)   | 2 (1%)   | 17          | 57  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 37  | d     | 203/205 (99%)   | 183 (90%)  | 20 (10%) | 0        | 100         | 100 |
| 38  | e     | 155/157 (99%)   | 137 (88%)  | 15 (10%) | 3 (2%)   | 9           | 46  |
| 39  | f     | 98/100 (98%)    | 81 (83%)   | 15 (15%) | 2 (2%)   | 8           | 45  |
| 40  | g     | 149/151 (99%)   | 136 (91%)  | 13 (9%)  | 0        | 100         | 100 |
| 41  | h     | 127/129 (98%)   | 122 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 42  | i     | 125/127 (98%)   | 109 (87%)  | 15 (12%) | 1 (1%)   | 21          | 62  |
| 43  | j     | 96/98 (98%)     | 81 (84%)   | 15 (16%) | 0        | 100         | 100 |
| 44  | k     | 114/116 (98%)   | 103 (90%)  | 11 (10%) | 0        | 100         | 100 |
| 45  | l     | 121/123 (98%)   | 97 (80%)   | 23 (19%) | 1 (1%)   | 21          | 62  |
| 46  | m     | 112/114 (98%)   | 99 (88%)   | 13 (12%) | 0        | 100         | 100 |
| 47  | n     | 99/101 (98%)    | 89 (90%)   | 10 (10%) | 0        | 100         | 100 |
| 48  | o     | 86/88 (98%)     | 77 (90%)   | 9 (10%)  | 0        | 100         | 100 |
| 49  | p     | 80/82 (98%)     | 73 (91%)   | 7 (9%)   | 0        | 100         | 100 |
| 50  | q     | 78/80 (98%)     | 66 (85%)   | 11 (14%) | 1 (1%)   | 13          | 53  |
| 51  | r     | 63/65 (97%)     | 59 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 52  | s     | 77/79 (98%)     | 74 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 53  | t     | 83/85 (98%)     | 79 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 54  | u     | 63/65 (97%)     | 51 (81%)   | 11 (18%) | 1 (2%)   | 11          | 49  |
| 55  | v     | 346/350 (99%)   | 322 (93%)  | 21 (6%)  | 3 (1%)   | 19          | 59  |
| 56  | w     | 492/529 (93%)   | 429 (87%)  | 55 (11%) | 8 (2%)   | 11          | 49  |
| 58  | z     | 12/14 (86%)     | 11 (92%)   | 0        | 1 (8%)   | 1           | 15  |
| All | All   | 6633/6776 (98%) | 6065 (91%) | 534 (8%) | 34 (0%)  | 35          | 71  |

All (34) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 46  | ASP  |
| 13  | M     | 58  | LYS  |
| 30  | 3     | 31  | ILE  |
| 36  | c     | 96  | VAL  |
| 50  | q     | 69  | THR  |
| 56  | w     | 315 | VAL  |
| 56  | w     | 395 | PRO  |
| 56  | w     | 400 | ARG  |
| 56  | w     | 472 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | w     | 503 | TYR  |
| 7   | G     | 47  | ASN  |
| 30  | 3     | 32  | LEU  |
| 38  | e     | 122 | VAL  |
| 39  | f     | 53  | LYS  |
| 45  | l     | 102 | ASP  |
| 55  | v     | 120 | GLY  |
| 55  | v     | 323 | ASN  |
| 56  | w     | 392 | ASN  |
| 21  | U     | 89  | GLY  |
| 39  | f     | 55  | HIS  |
| 54  | u     | 37  | TYR  |
| 56  | w     | 18  | ILE  |
| 55  | v     | 72  | PRO  |
| 12  | L     | 128 | THR  |
| 13  | M     | 59  | ARG  |
| 19  | S     | 64  | ALA  |
| 36  | c     | 97  | PRO  |
| 38  | e     | 121 | ASN  |
| 56  | w     | 77  | PHE  |
| 7   | G     | 174 | LYS  |
| 35  | b     | 17  | HIS  |
| 42  | i     | 90  | ASP  |
| 58  | z     | 16  | PRO  |
| 38  | e     | 97  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3   | C     | 216/216 (100%) | 214 (99%)  | 2 (1%)   | 81          | 90  |
| 4   | D     | 164/164 (100%) | 163 (99%)  | 1 (1%)   | 87          | 94  |
| 5   | E     | 165/165 (100%) | 164 (99%)  | 1 (1%)   | 87          | 94  |
| 6   | F     | 148/148 (100%) | 147 (99%)  | 1 (1%)   | 85          | 93  |
| 7   | G     | 137/137 (100%) | 137 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 8   | H     | 114/114 (100%) | 114 (100%) | 0        | 100         | 100 |
| 9   | I     | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 10  | J     | 116/116 (100%) | 116 (100%) | 0        | 100         | 100 |
| 11  | K     | 103/103 (100%) | 103 (100%) | 0        | 100         | 100 |
| 12  | L     | 102/102 (100%) | 102 (100%) | 0        | 100         | 100 |
| 13  | M     | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 14  | N     | 100/100 (100%) | 99 (99%)   | 1 (1%)   | 78          | 89  |
| 15  | O     | 86/86 (100%)   | 86 (100%)  | 0        | 100         | 100 |
| 16  | P     | 99/99 (100%)   | 99 (100%)  | 0        | 100         | 100 |
| 17  | Q     | 89/89 (100%)   | 89 (100%)  | 0        | 100         | 100 |
| 18  | R     | 84/84 (100%)   | 83 (99%)   | 1 (1%)   | 74          | 87  |
| 19  | S     | 93/93 (100%)   | 92 (99%)   | 1 (1%)   | 76          | 88  |
| 20  | T     | 80/80 (100%)   | 80 (100%)  | 0        | 100         | 100 |
| 21  | U     | 83/83 (100%)   | 83 (100%)  | 0        | 100         | 100 |
| 22  | V     | 78/78 (100%)   | 78 (100%)  | 0        | 100         | 100 |
| 23  | W     | 57/57 (100%)   | 56 (98%)   | 1 (2%)   | 62          | 83  |
| 24  | X     | 67/67 (100%)   | 66 (98%)   | 1 (2%)   | 67          | 85  |
| 25  | Y     | 55/55 (100%)   | 55 (100%)  | 0        | 100         | 100 |
| 26  | Z     | 48/48 (100%)   | 48 (100%)  | 0        | 100         | 100 |
| 27  | 0     | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 28  | 1     | 45/45 (100%)   | 45 (100%)  | 0        | 100         | 100 |
| 29  | 2     | 38/38 (100%)   | 38 (100%)  | 0        | 100         | 100 |
| 30  | 3     | 51/51 (100%)   | 51 (100%)  | 0        | 100         | 100 |
| 31  | 4     | 34/34 (100%)   | 33 (97%)   | 1 (3%)   | 45          | 72  |
| 32  | 5     | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 35  | b     | 180/180 (100%) | 177 (98%)  | 3 (2%)   | 63          | 83  |
| 36  | c     | 170/170 (100%) | 170 (100%) | 0        | 100         | 100 |
| 37  | d     | 172/172 (100%) | 170 (99%)  | 2 (1%)   | 74          | 87  |
| 38  | e     | 114/119 (96%)  | 113 (99%)  | 1 (1%)   | 81          | 90  |
| 39  | f     | 87/87 (100%)   | 87 (100%)  | 0        | 100         | 100 |
| 40  | g     | 124/124 (100%) | 123 (99%)  | 1 (1%)   | 83          | 91  |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 41  | h     | 104/104 (100%)  | 104 (100%)  | 0        | 100         | 100 |
| 42  | i     | 105/105 (100%)  | 104 (99%)   | 1 (1%)   | 78          | 89  |
| 43  | j     | 86/86 (100%)    | 86 (100%)   | 0        | 100         | 100 |
| 44  | k     | 89/89 (100%)    | 88 (99%)    | 1 (1%)   | 76          | 88  |
| 45  | l     | 103/103 (100%)  | 103 (100%)  | 0        | 100         | 100 |
| 46  | m     | 92/92 (100%)    | 91 (99%)    | 1 (1%)   | 76          | 88  |
| 47  | n     | 79/83 (95%)     | 79 (100%)   | 0        | 100         | 100 |
| 48  | o     | 76/76 (100%)    | 76 (100%)   | 0        | 100         | 100 |
| 49  | p     | 65/65 (100%)    | 65 (100%)   | 0        | 100         | 100 |
| 50  | q     | 74/74 (100%)    | 73 (99%)    | 1 (1%)   | 69          | 86  |
| 51  | r     | 48/56 (86%)     | 48 (100%)   | 0        | 100         | 100 |
| 52  | s     | 70/70 (100%)    | 70 (100%)   | 0        | 100         | 100 |
| 53  | t     | 65/65 (100%)    | 65 (100%)   | 0        | 100         | 100 |
| 54  | u     | 44/55 (80%)     | 44 (100%)   | 0        | 100         | 100 |
| 55  | v     | 203/292 (70%)   | 201 (99%)   | 2 (1%)   | 78          | 89  |
| 56  | w     | 426/453 (94%)   | 422 (99%)   | 4 (1%)   | 81          | 90  |
| 58  | z     | 14/14 (100%)    | 14 (100%)   | 0        | 100         | 100 |
| All | All   | 5407/5551 (97%) | 5379 (100%) | 28 (0%)  | 90          | 95  |

All (28) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 36  | ASN  |
| 3   | C     | 85  | ASN  |
| 4   | D     | 33  | ARG  |
| 5   | E     | 156 | ASN  |
| 6   | F     | 176 | PHE  |
| 14  | N     | 2   | ARG  |
| 18  | R     | 43  | ASN  |
| 19  | S     | 57  | ASN  |
| 23  | W     | 51  | ARG  |
| 24  | X     | 26  | ARG  |
| 31  | 4     | 36  | ARG  |
| 35  | b     | 23  | ASN  |
| 35  | b     | 35  | ASN  |
| 35  | b     | 202 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | d     | 80  | ARG  |
| 37  | d     | 177 | MET  |
| 38  | e     | 69  | ASN  |
| 40  | g     | 142 | ARG  |
| 42  | i     | 44  | ARG  |
| 44  | k     | 12  | ARG  |
| 46  | m     | 7   | ASN  |
| 50  | q     | 61  | ARG  |
| 55  | v     | 236 | HIS  |
| 55  | v     | 238 | ASN  |
| 56  | w     | 71  | THR  |
| 56  | w     | 124 | ARG  |
| 56  | w     | 125 | LYS  |
| 56  | w     | 152 | MET  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 36  | ASN  |
| 3   | C     | 85  | ASN  |
| 3   | C     | 114 | GLN  |
| 3   | C     | 250 | GLN  |
| 4   | D     | 150 | GLN  |
| 5   | E     | 156 | ASN  |
| 7   | G     | 63  | GLN  |
| 14  | N     | 9   | GLN  |
| 15  | O     | 38  | GLN  |
| 16  | P     | 11  | GLN  |
| 16  | P     | 55  | HIS  |
| 17  | Q     | 43  | GLN  |
| 18  | R     | 6   | GLN  |
| 18  | R     | 18  | GLN  |
| 18  | R     | 43  | ASN  |
| 19  | S     | 7   | HIS  |
| 19  | S     | 57  | ASN  |
| 22  | V     | 87  | GLN  |
| 25  | Y     | 58  | ASN  |
| 32  | 5     | 4   | ASN  |
| 35  | b     | 23  | ASN  |
| 35  | b     | 35  | ASN  |
| 37  | d     | 115 | GLN  |
| 38  | e     | 69  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | f     | 11  | HIS  |
| 39  | f     | 58  | HIS  |
| 41  | h     | 3   | GLN  |
| 41  | h     | 75  | GLN  |
| 42  | i     | 4   | GLN  |
| 42  | i     | 36  | GLN  |
| 42  | i     | 74  | GLN  |
| 43  | j     | 58  | ASN  |
| 44  | k     | 100 | ASN  |
| 44  | k     | 117 | HIS  |
| 48  | o     | 45  | HIS  |
| 49  | p     | 18  | GLN  |
| 49  | p     | 63  | GLN  |
| 50  | q     | 30  | HIS  |
| 51  | r     | 51  | GLN  |
| 53  | t     | 2   | ASN  |
| 55  | v     | 197 | HIS  |
| 55  | v     | 235 | GLN  |
| 55  | v     | 236 | HIS  |
| 55  | v     | 263 | GLN  |
| 55  | v     | 296 | ASN  |
| 56  | w     | 311 | HIS  |
| 56  | w     | 381 | GLN  |
| 56  | w     | 418 | GLN  |
| 56  | w     | 445 | GLN  |
| 56  | w     | 510 | ASN  |
| 56  | w     | 525 | GLN  |
| 58  | z     | 15  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 2893/2903 (99%) | 533 (18%)         | 30 (1%)         |
| 2   | B     | 119/120 (99%)   | 14 (11%)          | 2 (1%)          |
| 33  | 7     | 6/7 (85%)       | 5 (83%)           | 0               |
| 34  | a     | 1538/1539 (99%) | 219 (14%)         | 0               |
| 57  | x     | 76/77 (98%)     | 21 (27%)          | 0               |
| All | All   | 4632/4646 (99%) | 792 (17%)         | 32 (0%)         |

All (792) RNA backbone outliers are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | U    |
| 1   | A     | 14  | A    |
| 1   | A     | 27  | G    |
| 1   | A     | 34  | U    |
| 1   | A     | 35  | G    |
| 1   | A     | 36  | G    |
| 1   | A     | 46  | G    |
| 1   | A     | 49  | A    |
| 1   | A     | 51  | G    |
| 1   | A     | 52  | A    |
| 1   | A     | 60  | G    |
| 1   | A     | 63  | A    |
| 1   | A     | 71  | A    |
| 1   | A     | 74  | A    |
| 1   | A     | 75  | G    |
| 1   | A     | 84  | A    |
| 1   | A     | 91  | A    |
| 1   | A     | 92  | U    |
| 1   | A     | 98  | G    |
| 1   | A     | 110 | G    |
| 1   | A     | 118 | A    |
| 1   | A     | 119 | A    |
| 1   | A     | 120 | U    |
| 1   | A     | 125 | A    |
| 1   | A     | 139 | U    |
| 1   | A     | 140 | C    |
| 1   | A     | 141 | G    |
| 1   | A     | 142 | A    |
| 1   | A     | 158 | U    |
| 1   | A     | 162 | U    |
| 1   | A     | 163 | C    |
| 1   | A     | 188 | G    |
| 1   | A     | 196 | A    |
| 1   | A     | 199 | A    |
| 1   | A     | 205 | G    |
| 1   | A     | 206 | U    |
| 1   | A     | 215 | G    |
| 1   | A     | 216 | A    |
| 1   | A     | 218 | A    |
| 1   | A     | 219 | A    |
| 1   | A     | 221 | A    |
| 1   | A     | 222 | A    |
| 1   | A     | 223 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 242 | G    |
| 1   | A     | 243 | U    |
| 1   | A     | 248 | G    |
| 1   | A     | 249 | C    |
| 1   | A     | 250 | G    |
| 1   | A     | 255 | A    |
| 1   | A     | 266 | G    |
| 1   | A     | 267 | C    |
| 1   | A     | 276 | U    |
| 1   | A     | 278 | A    |
| 1   | A     | 281 | C    |
| 1   | A     | 294 | A    |
| 1   | A     | 310 | A    |
| 1   | A     | 311 | A    |
| 1   | A     | 323 | C    |
| 1   | A     | 324 | A    |
| 1   | A     | 329 | G    |
| 1   | A     | 330 | A    |
| 1   | A     | 334 | C    |
| 1   | A     | 343 | C    |
| 1   | A     | 361 | G    |
| 1   | A     | 367 | G    |
| 1   | A     | 371 | A    |
| 1   | A     | 372 | G    |
| 1   | A     | 373 | U    |
| 1   | A     | 386 | G    |
| 1   | A     | 387 | U    |
| 1   | A     | 404 | A    |
| 1   | A     | 406 | G    |
| 1   | A     | 411 | G    |
| 1   | A     | 417 | C    |
| 1   | A     | 421 | C    |
| 1   | A     | 424 | G    |
| 1   | A     | 451 | U    |
| 1   | A     | 455 | C    |
| 1   | A     | 456 | C    |
| 1   | A     | 457 | A    |
| 1   | A     | 458 | G    |
| 1   | A     | 459 | U    |
| 1   | A     | 467 | G    |
| 1   | A     | 480 | A    |
| 1   | A     | 481 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 489 | G    |
| 1   | A     | 490 | C    |
| 1   | A     | 491 | G    |
| 1   | A     | 504 | A    |
| 1   | A     | 505 | A    |
| 1   | A     | 506 | G    |
| 1   | A     | 509 | C    |
| 1   | A     | 528 | A    |
| 1   | A     | 529 | A    |
| 1   | A     | 530 | G    |
| 1   | A     | 532 | A    |
| 1   | A     | 533 | G    |
| 1   | A     | 543 | G    |
| 1   | A     | 544 | C    |
| 1   | A     | 545 | U    |
| 1   | A     | 547 | A    |
| 1   | A     | 548 | G    |
| 1   | A     | 550 | C    |
| 1   | A     | 555 | G    |
| 1   | A     | 563 | A    |
| 1   | A     | 568 | U    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | U    |
| 1   | A     | 575 | A    |
| 1   | A     | 603 | A    |
| 1   | A     | 616 | A    |
| 1   | A     | 621 | A    |
| 1   | A     | 627 | A    |
| 1   | A     | 637 | A    |
| 1   | A     | 643 | A    |
| 1   | A     | 645 | C    |
| 1   | A     | 646 | U    |
| 1   | A     | 654 | A    |
| 1   | A     | 668 | A    |
| 1   | A     | 669 | G    |
| 1   | A     | 670 | A    |
| 1   | A     | 677 | A    |
| 1   | A     | 686 | U    |
| 1   | A     | 687 | C    |
| 1   | A     | 695 | G    |
| 1   | A     | 704 | G    |
| 1   | A     | 711 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 717 | C    |
| 1   | A     | 726 | G    |
| 1   | A     | 729 | G    |
| 1   | A     | 730 | A    |
| 1   | A     | 745 | G    |
| 1   | A     | 747 | C    |
| 1   | A     | 752 | A    |
| 1   | A     | 753 | A    |
| 1   | A     | 763 | G    |
| 1   | A     | 764 | A    |
| 1   | A     | 765 | C    |
| 1   | A     | 774 | G    |
| 1   | A     | 775 | G    |
| 1   | A     | 776 | G    |
| 1   | A     | 777 | G    |
| 1   | A     | 782 | A    |
| 1   | A     | 784 | G    |
| 1   | A     | 785 | G    |
| 1   | A     | 789 | A    |
| 1   | A     | 800 | A    |
| 1   | A     | 805 | G    |
| 1   | A     | 811 | U    |
| 1   | A     | 812 | C    |
| 1   | A     | 819 | A    |
| 1   | A     | 822 | G    |
| 1   | A     | 827 | U    |
| 1   | A     | 828 | U    |
| 1   | A     | 830 | G    |
| 1   | A     | 831 | G    |
| 1   | A     | 845 | A    |
| 1   | A     | 846 | U    |
| 1   | A     | 847 | U    |
| 1   | A     | 856 | G    |
| 1   | A     | 858 | G    |
| 1   | A     | 859 | G    |
| 1   | A     | 860 | U    |
| 1   | A     | 869 | G    |
| 1   | A     | 878 | A    |
| 1   | A     | 896 | A    |
| 1   | A     | 897 | C    |
| 1   | A     | 898 | C    |
| 1   | A     | 904 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 907  | G    |
| 1   | A     | 910  | A    |
| 1   | A     | 932  | U    |
| 1   | A     | 941  | A    |
| 1   | A     | 946  | C    |
| 1   | A     | 953  | G    |
| 1   | A     | 961  | C    |
| 1   | A     | 965  | C    |
| 1   | A     | 974  | G    |
| 1   | A     | 980  | A    |
| 1   | A     | 983  | A    |
| 1   | A     | 989  | G    |
| 1   | A     | 995  | C    |
| 1   | A     | 996  | A    |
| 1   | A     | 999  | U    |
| 1   | A     | 1010 | A    |
| 1   | A     | 1012 | U    |
| 1   | A     | 1013 | C    |
| 1   | A     | 1021 | A    |
| 1   | A     | 1023 | U    |
| 1   | A     | 1026 | G    |
| 1   | A     | 1033 | U    |
| 1   | A     | 1046 | A    |
| 1   | A     | 1047 | G    |
| 1   | A     | 1053 | C    |
| 1   | A     | 1057 | A    |
| 1   | A     | 1059 | G    |
| 1   | A     | 1060 | U    |
| 1   | A     | 1061 | U    |
| 1   | A     | 1062 | G    |
| 1   | A     | 1064 | C    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1066 | U    |
| 1   | A     | 1068 | G    |
| 1   | A     | 1069 | A    |
| 1   | A     | 1070 | A    |
| 1   | A     | 1071 | G    |
| 1   | A     | 1072 | C    |
| 1   | A     | 1075 | C    |
| 1   | A     | 1076 | C    |
| 1   | A     | 1078 | U    |
| 1   | A     | 1079 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1083 | U    |
| 1   | A     | 1084 | A    |
| 1   | A     | 1088 | A    |
| 1   | A     | 1104 | C    |
| 1   | A     | 1106 | G    |
| 1   | A     | 1111 | A    |
| 1   | A     | 1112 | G    |
| 1   | A     | 1130 | U    |
| 1   | A     | 1131 | G    |
| 1   | A     | 1132 | U    |
| 1   | A     | 1133 | A    |
| 1   | A     | 1135 | C    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1142 | A    |
| 1   | A     | 1157 | G    |
| 1   | A     | 1172 | C    |
| 1   | A     | 1174 | U    |
| 1   | A     | 1176 | U    |
| 1   | A     | 1177 | G    |
| 1   | A     | 1178 | C    |
| 1   | A     | 1180 | U    |
| 1   | A     | 1204 | A    |
| 1   | A     | 1206 | G    |
| 1   | A     | 1211 | C    |
| 1   | A     | 1212 | G    |
| 1   | A     | 1225 | G    |
| 1   | A     | 1237 | A    |
| 1   | A     | 1247 | A    |
| 1   | A     | 1248 | G    |
| 1   | A     | 1250 | G    |
| 1   | A     | 1251 | C    |
| 1   | A     | 1253 | A    |
| 1   | A     | 1256 | G    |
| 1   | A     | 1271 | G    |
| 1   | A     | 1272 | A    |
| 1   | A     | 1289 | C    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1301 | A    |
| 1   | A     | 1315 | C    |
| 1   | A     | 1321 | A    |
| 1   | A     | 1325 | U    |
| 1   | A     | 1329 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1330 | C    |
| 1   | A     | 1341 | G    |
| 1   | A     | 1345 | C    |
| 1   | A     | 1365 | A    |
| 1   | A     | 1368 | G    |
| 1   | A     | 1378 | A    |
| 1   | A     | 1379 | U    |
| 1   | A     | 1383 | A    |
| 1   | A     | 1395 | A    |
| 1   | A     | 1416 | G    |
| 1   | A     | 1419 | A    |
| 1   | A     | 1420 | A    |
| 1   | A     | 1421 | G    |
| 1   | A     | 1428 | C    |
| 1   | A     | 1437 | C    |
| 1   | A     | 1454 | C    |
| 1   | A     | 1461 | C    |
| 1   | A     | 1475 | G    |
| 1   | A     | 1482 | G    |
| 1   | A     | 1490 | A    |
| 1   | A     | 1491 | G    |
| 1   | A     | 1493 | C    |
| 1   | A     | 1504 | A    |
| 1   | A     | 1515 | A    |
| 1   | A     | 1524 | G    |
| 1   | A     | 1532 | A    |
| 1   | A     | 1533 | C    |
| 1   | A     | 1535 | A    |
| 1   | A     | 1536 | C    |
| 1   | A     | 1537 | G    |
| 1   | A     | 1555 | G    |
| 1   | A     | 1559 | U    |
| 1   | A     | 1560 | G    |
| 1   | A     | 1565 | C    |
| 1   | A     | 1569 | A    |
| 1   | A     | 1578 | U    |
| 1   | A     | 1585 | C    |
| 1   | A     | 1598 | A    |
| 1   | A     | 1603 | A    |
| 1   | A     | 1607 | C    |
| 1   | A     | 1610 | A    |
| 1   | A     | 1611 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1634 | A    |
| 1   | A     | 1646 | C    |
| 1   | A     | 1647 | U    |
| 1   | A     | 1648 | U    |
| 1   | A     | 1651 | G    |
| 1   | A     | 1660 | G    |
| 1   | A     | 1664 | A    |
| 1   | A     | 1665 | A    |
| 1   | A     | 1669 | A    |
| 1   | A     | 1670 | C    |
| 1   | A     | 1674 | G    |
| 1   | A     | 1694 | C    |
| 1   | A     | 1695 | G    |
| 1   | A     | 1715 | G    |
| 1   | A     | 1729 | U    |
| 1   | A     | 1730 | C    |
| 1   | A     | 1732 | C    |
| 1   | A     | 1733 | G    |
| 1   | A     | 1738 | G    |
| 1   | A     | 1757 | A    |
| 1   | A     | 1758 | U    |
| 1   | A     | 1764 | C    |
| 1   | A     | 1773 | A    |
| 1   | A     | 1780 | A    |
| 1   | A     | 1781 | U    |
| 1   | A     | 1782 | U    |
| 1   | A     | 1784 | A    |
| 1   | A     | 1800 | C    |
| 1   | A     | 1801 | A    |
| 1   | A     | 1802 | A    |
| 1   | A     | 1808 | A    |
| 1   | A     | 1816 | C    |
| 1   | A     | 1829 | A    |
| 1   | A     | 1833 | C    |
| 1   | A     | 1835 | G    |
| 1   | A     | 1847 | G    |
| 1   | A     | 1848 | A    |
| 1   | A     | 1870 | C    |
| 1   | A     | 1871 | A    |
| 1   | A     | 1873 | G    |
| 1   | A     | 1896 | G    |
| 1   | A     | 1901 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1906 | G    |
| 1   | A     | 1907 | G    |
| 1   | A     | 1913 | A    |
| 1   | A     | 1914 | C    |
| 1   | A     | 1915 | U    |
| 1   | A     | 1917 | U    |
| 1   | A     | 1927 | A    |
| 1   | A     | 1929 | G    |
| 1   | A     | 1930 | G    |
| 1   | A     | 1937 | A    |
| 1   | A     | 1938 | A    |
| 1   | A     | 1940 | U    |
| 1   | A     | 1941 | C    |
| 1   | A     | 1944 | U    |
| 1   | A     | 1955 | U    |
| 1   | A     | 1960 | A    |
| 1   | A     | 1962 | C    |
| 1   | A     | 1963 | U    |
| 1   | A     | 1967 | C    |
| 1   | A     | 1970 | A    |
| 1   | A     | 1971 | U    |
| 1   | A     | 1972 | G    |
| 1   | A     | 1991 | U    |
| 1   | A     | 1992 | G    |
| 1   | A     | 1997 | C    |
| 1   | A     | 2020 | A    |
| 1   | A     | 2022 | U    |
| 1   | A     | 2023 | C    |
| 1   | A     | 2030 | A    |
| 1   | A     | 2031 | A    |
| 1   | A     | 2033 | A    |
| 1   | A     | 2043 | C    |
| 1   | A     | 2050 | C    |
| 1   | A     | 2052 | A    |
| 1   | A     | 2055 | C    |
| 1   | A     | 2056 | G    |
| 1   | A     | 2060 | A    |
| 1   | A     | 2061 | G    |
| 1   | A     | 2062 | A    |
| 1   | A     | 2068 | U    |
| 1   | A     | 2069 | G    |
| 1   | A     | 2072 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2093 | G    |
| 1   | A     | 2096 | C    |
| 1   | A     | 2100 | G    |
| 1   | A     | 2108 | A    |
| 1   | A     | 2110 | G    |
| 1   | A     | 2111 | U    |
| 1   | A     | 2112 | G    |
| 1   | A     | 2113 | U    |
| 1   | A     | 2118 | U    |
| 1   | A     | 2119 | A    |
| 1   | A     | 2127 | G    |
| 1   | A     | 2131 | U    |
| 1   | A     | 2132 | U    |
| 1   | A     | 2133 | G    |
| 1   | A     | 2136 | G    |
| 1   | A     | 2145 | C    |
| 1   | A     | 2147 | A    |
| 1   | A     | 2157 | G    |
| 1   | A     | 2162 | G    |
| 1   | A     | 2164 | C    |
| 1   | A     | 2170 | A    |
| 1   | A     | 2172 | U    |
| 1   | A     | 2173 | A    |
| 1   | A     | 2178 | C    |
| 1   | A     | 2189 | U    |
| 1   | A     | 2192 | U    |
| 1   | A     | 2198 | A    |
| 1   | A     | 2204 | G    |
| 1   | A     | 2211 | A    |
| 1   | A     | 2212 | A    |
| 1   | A     | 2213 | U    |
| 1   | A     | 2225 | A    |
| 1   | A     | 2238 | G    |
| 1   | A     | 2239 | G    |
| 1   | A     | 2249 | U    |
| 1   | A     | 2250 | G    |
| 1   | A     | 2251 | G    |
| 1   | A     | 2279 | G    |
| 1   | A     | 2283 | C    |
| 1   | A     | 2287 | A    |
| 1   | A     | 2297 | A    |
| 1   | A     | 2305 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2309 | A    |
| 1   | A     | 2325 | G    |
| 1   | A     | 2327 | A    |
| 1   | A     | 2334 | U    |
| 1   | A     | 2335 | A    |
| 1   | A     | 2336 | A    |
| 1   | A     | 2345 | G    |
| 1   | A     | 2350 | C    |
| 1   | A     | 2354 | C    |
| 1   | A     | 2357 | G    |
| 1   | A     | 2361 | G    |
| 1   | A     | 2383 | G    |
| 1   | A     | 2385 | C    |
| 1   | A     | 2391 | G    |
| 1   | A     | 2392 | A    |
| 1   | A     | 2402 | U    |
| 1   | A     | 2407 | A    |
| 1   | A     | 2423 | U    |
| 1   | A     | 2424 | C    |
| 1   | A     | 2426 | A    |
| 1   | A     | 2427 | C    |
| 1   | A     | 2428 | G    |
| 1   | A     | 2429 | G    |
| 1   | A     | 2430 | A    |
| 1   | A     | 2435 | A    |
| 1   | A     | 2441 | U    |
| 1   | A     | 2447 | G    |
| 1   | A     | 2448 | A    |
| 1   | A     | 2449 | U    |
| 1   | A     | 2473 | U    |
| 1   | A     | 2476 | A    |
| 1   | A     | 2484 | G    |
| 1   | A     | 2491 | U    |
| 1   | A     | 2494 | G    |
| 1   | A     | 2498 | C    |
| 1   | A     | 2502 | G    |
| 1   | A     | 2503 | A    |
| 1   | A     | 2504 | U    |
| 1   | A     | 2506 | U    |
| 1   | A     | 2513 | A    |
| 1   | A     | 2518 | A    |
| 1   | A     | 2520 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2529 | G    |
| 1   | A     | 2531 | A    |
| 1   | A     | 2535 | G    |
| 1   | A     | 2547 | A    |
| 1   | A     | 2554 | U    |
| 1   | A     | 2564 | A    |
| 1   | A     | 2567 | G    |
| 1   | A     | 2572 | A    |
| 1   | A     | 2573 | C    |
| 1   | A     | 2580 | U    |
| 1   | A     | 2582 | G    |
| 1   | A     | 2585 | U    |
| 1   | A     | 2586 | U    |
| 1   | A     | 2602 | A    |
| 1   | A     | 2603 | G    |
| 1   | A     | 2605 | U    |
| 1   | A     | 2609 | U    |
| 1   | A     | 2613 | U    |
| 1   | A     | 2614 | A    |
| 1   | A     | 2621 | G    |
| 1   | A     | 2629 | U    |
| 1   | A     | 2634 | A    |
| 1   | A     | 2636 | C    |
| 1   | A     | 2646 | C    |
| 1   | A     | 2654 | A    |
| 1   | A     | 2655 | G    |
| 1   | A     | 2656 | U    |
| 1   | A     | 2673 | G    |
| 1   | A     | 2682 | A    |
| 1   | A     | 2689 | U    |
| 1   | A     | 2690 | U    |
| 1   | A     | 2712 | C    |
| 1   | A     | 2713 | U    |
| 1   | A     | 2714 | G    |
| 1   | A     | 2716 | C    |
| 1   | A     | 2718 | G    |
| 1   | A     | 2722 | G    |
| 1   | A     | 2726 | A    |
| 1   | A     | 2731 | G    |
| 1   | A     | 2733 | A    |
| 1   | A     | 2744 | G    |
| 1   | A     | 2748 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2751 | G    |
| 1   | A     | 2762 | C    |
| 1   | A     | 2764 | A    |
| 1   | A     | 2765 | A    |
| 1   | A     | 2778 | A    |
| 1   | A     | 2779 | U    |
| 1   | A     | 2791 | G    |
| 1   | A     | 2794 | C    |
| 1   | A     | 2796 | U    |
| 1   | A     | 2797 | U    |
| 1   | A     | 2799 | A    |
| 1   | A     | 2800 | A    |
| 1   | A     | 2808 | G    |
| 1   | A     | 2809 | A    |
| 1   | A     | 2818 | U    |
| 1   | A     | 2820 | A    |
| 1   | A     | 2833 | U    |
| 1   | A     | 2834 | G    |
| 1   | A     | 2835 | A    |
| 1   | A     | 2849 | U    |
| 1   | A     | 2861 | U    |
| 1   | A     | 2867 | G    |
| 1   | A     | 2868 | A    |
| 1   | A     | 2872 | A    |
| 1   | A     | 2873 | A    |
| 1   | A     | 2880 | C    |
| 1   | A     | 2884 | U    |
| 1   | A     | 2902 | C    |
| 2   | B     | 4    | C    |
| 2   | B     | 9    | G    |
| 2   | B     | 13   | G    |
| 2   | B     | 35   | C    |
| 2   | B     | 41   | G    |
| 2   | B     | 44   | G    |
| 2   | B     | 45   | A    |
| 2   | B     | 53   | A    |
| 2   | B     | 67   | G    |
| 2   | B     | 89   | U    |
| 2   | B     | 90   | C    |
| 2   | B     | 91   | C    |
| 2   | B     | 108  | A    |
| 2   | B     | 109  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | 7     | 27  | G    |
| 33  | 7     | 28  | U    |
| 33  | 7     | 29  | A    |
| 33  | 7     | 30  | A    |
| 33  | 7     | 31  | A    |
| 34  | a     | 7   | A    |
| 34  | a     | 9   | G    |
| 34  | a     | 22  | G    |
| 34  | a     | 32  | A    |
| 34  | a     | 39  | G    |
| 34  | a     | 47  | C    |
| 34  | a     | 48  | C    |
| 34  | a     | 49  | U    |
| 34  | a     | 51  | A    |
| 34  | a     | 71  | A    |
| 34  | a     | 81  | A    |
| 34  | a     | 86  | G    |
| 34  | a     | 94  | G    |
| 34  | a     | 95  | C    |
| 34  | a     | 121 | U    |
| 34  | a     | 130 | A    |
| 34  | a     | 163 | C    |
| 34  | a     | 173 | U    |
| 34  | a     | 174 | A    |
| 34  | a     | 177 | G    |
| 34  | a     | 181 | A    |
| 34  | a     | 183 | C    |
| 34  | a     | 184 | G    |
| 34  | a     | 197 | A    |
| 34  | a     | 209 | U    |
| 34  | a     | 210 | C    |
| 34  | a     | 211 | G    |
| 34  | a     | 212 | G    |
| 34  | a     | 226 | G    |
| 34  | a     | 240 | G    |
| 34  | a     | 247 | G    |
| 34  | a     | 251 | G    |
| 34  | a     | 266 | G    |
| 34  | a     | 267 | C    |
| 34  | a     | 269 | C    |
| 34  | a     | 279 | A    |
| 34  | a     | 280 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | a     | 281 | G    |
| 34  | a     | 283 | U    |
| 34  | a     | 289 | G    |
| 34  | a     | 306 | A    |
| 34  | a     | 328 | C    |
| 34  | a     | 344 | A    |
| 34  | a     | 345 | C    |
| 34  | a     | 346 | G    |
| 34  | a     | 347 | G    |
| 34  | a     | 351 | G    |
| 34  | a     | 352 | C    |
| 34  | a     | 354 | G    |
| 34  | a     | 356 | A    |
| 34  | a     | 367 | U    |
| 34  | a     | 372 | C    |
| 34  | a     | 388 | G    |
| 34  | a     | 392 | C    |
| 34  | a     | 397 | A    |
| 34  | a     | 406 | G    |
| 34  | a     | 411 | A    |
| 34  | a     | 413 | G    |
| 34  | a     | 421 | U    |
| 34  | a     | 422 | C    |
| 34  | a     | 424 | G    |
| 34  | a     | 429 | U    |
| 34  | a     | 439 | U    |
| 34  | a     | 467 | U    |
| 34  | a     | 479 | U    |
| 34  | a     | 482 | A    |
| 34  | a     | 484 | G    |
| 34  | a     | 486 | U    |
| 34  | a     | 496 | A    |
| 34  | a     | 497 | G    |
| 34  | a     | 509 | A    |
| 34  | a     | 510 | A    |
| 34  | a     | 511 | C    |
| 34  | a     | 516 | U    |
| 34  | a     | 518 | C    |
| 34  | a     | 519 | C    |
| 34  | a     | 521 | G    |
| 34  | a     | 527 | G    |
| 34  | a     | 531 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | a     | 532 | A    |
| 34  | a     | 536 | C    |
| 34  | a     | 547 | A    |
| 34  | a     | 560 | A    |
| 34  | a     | 561 | U    |
| 34  | a     | 564 | C    |
| 34  | a     | 572 | A    |
| 34  | a     | 573 | A    |
| 34  | a     | 574 | A    |
| 34  | a     | 575 | G    |
| 34  | a     | 576 | C    |
| 34  | a     | 577 | G    |
| 34  | a     | 596 | A    |
| 34  | a     | 633 | G    |
| 34  | a     | 665 | A    |
| 34  | a     | 688 | G    |
| 34  | a     | 702 | A    |
| 34  | a     | 703 | G    |
| 34  | a     | 713 | G    |
| 34  | a     | 724 | G    |
| 34  | a     | 731 | G    |
| 34  | a     | 733 | G    |
| 34  | a     | 748 | G    |
| 34  | a     | 755 | G    |
| 34  | a     | 777 | A    |
| 34  | a     | 814 | A    |
| 34  | a     | 815 | A    |
| 34  | a     | 817 | C    |
| 34  | a     | 818 | G    |
| 34  | a     | 819 | A    |
| 34  | a     | 820 | U    |
| 34  | a     | 821 | G    |
| 34  | a     | 829 | G    |
| 34  | a     | 832 | G    |
| 34  | a     | 843 | U    |
| 34  | a     | 844 | G    |
| 34  | a     | 846 | G    |
| 34  | a     | 871 | U    |
| 34  | a     | 873 | A    |
| 34  | a     | 876 | C    |
| 34  | a     | 889 | A    |
| 34  | a     | 890 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | a     | 902  | G    |
| 34  | a     | 934  | C    |
| 34  | a     | 935  | A    |
| 34  | a     | 960  | U    |
| 34  | a     | 961  | U    |
| 34  | a     | 966  | G    |
| 34  | a     | 969  | A    |
| 34  | a     | 971  | G    |
| 34  | a     | 975  | A    |
| 34  | a     | 976  | G    |
| 34  | a     | 977  | A    |
| 34  | a     | 992  | U    |
| 34  | a     | 993  | G    |
| 34  | a     | 1004 | A    |
| 34  | a     | 1026 | G    |
| 34  | a     | 1028 | C    |
| 34  | a     | 1030 | U    |
| 34  | a     | 1031 | C    |
| 34  | a     | 1033 | G    |
| 34  | a     | 1034 | G    |
| 34  | a     | 1035 | A    |
| 34  | a     | 1056 | U    |
| 34  | a     | 1064 | G    |
| 34  | a     | 1065 | U    |
| 34  | a     | 1085 | U    |
| 34  | a     | 1094 | G    |
| 34  | a     | 1101 | A    |
| 34  | a     | 1108 | G    |
| 34  | a     | 1130 | A    |
| 34  | a     | 1136 | C    |
| 34  | a     | 1137 | C    |
| 34  | a     | 1138 | G    |
| 34  | a     | 1139 | G    |
| 34  | a     | 1152 | A    |
| 34  | a     | 1158 | C    |
| 34  | a     | 1159 | U    |
| 34  | a     | 1168 | U    |
| 34  | a     | 1183 | U    |
| 34  | a     | 1184 | G    |
| 34  | a     | 1191 | A    |
| 34  | a     | 1196 | A    |
| 34  | a     | 1197 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | a     | 1201 | A    |
| 34  | a     | 1202 | U    |
| 34  | a     | 1212 | U    |
| 34  | a     | 1213 | A    |
| 34  | a     | 1225 | A    |
| 34  | a     | 1227 | A    |
| 34  | a     | 1238 | A    |
| 34  | a     | 1240 | U    |
| 34  | a     | 1241 | G    |
| 34  | a     | 1253 | G    |
| 34  | a     | 1256 | A    |
| 34  | a     | 1258 | G    |
| 34  | a     | 1260 | G    |
| 34  | a     | 1278 | G    |
| 34  | a     | 1280 | A    |
| 34  | a     | 1281 | C    |
| 34  | a     | 1282 | C    |
| 34  | a     | 1287 | A    |
| 34  | a     | 1290 | G    |
| 34  | a     | 1298 | U    |
| 34  | a     | 1300 | G    |
| 34  | a     | 1301 | U    |
| 34  | a     | 1312 | G    |
| 34  | a     | 1317 | C    |
| 34  | a     | 1320 | C    |
| 34  | a     | 1340 | A    |
| 34  | a     | 1346 | A    |
| 34  | a     | 1347 | G    |
| 34  | a     | 1348 | U    |
| 34  | a     | 1363 | A    |
| 34  | a     | 1378 | C    |
| 34  | a     | 1395 | C    |
| 34  | a     | 1397 | C    |
| 34  | a     | 1398 | A    |
| 34  | a     | 1400 | C    |
| 34  | a     | 1401 | G    |
| 34  | a     | 1433 | A    |
| 34  | a     | 1446 | A    |
| 34  | a     | 1448 | C    |
| 34  | a     | 1451 | U    |
| 34  | a     | 1452 | C    |
| 34  | a     | 1492 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | a     | 1493 | A    |
| 34  | a     | 1494 | G    |
| 34  | a     | 1495 | U    |
| 34  | a     | 1499 | A    |
| 34  | a     | 1502 | A    |
| 34  | a     | 1503 | A    |
| 34  | a     | 1517 | G    |
| 34  | a     | 1520 | C    |
| 34  | a     | 1529 | G    |
| 34  | a     | 1530 | G    |
| 34  | a     | 1533 | C    |
| 34  | a     | 1534 | A    |
| 34  | a     | 1535 | C    |
| 34  | a     | 1536 | C    |
| 57  | x     | 8    | U    |
| 57  | x     | 9    | G    |
| 57  | x     | 13   | C    |
| 57  | x     | 14   | A    |
| 57  | x     | 19   | G    |
| 57  | x     | 20   | G    |
| 57  | x     | 21   | U    |
| 57  | x     | 22   | A    |
| 57  | x     | 26   | C    |
| 57  | x     | 47   | G    |
| 57  | x     | 49   | C    |
| 57  | x     | 58   | A    |
| 57  | x     | 59   | A    |
| 57  | x     | 61   | U    |
| 57  | x     | 68   | C    |
| 57  | x     | 69   | C    |
| 57  | x     | 71   | G    |
| 57  | x     | 72   | C    |
| 57  | x     | 73   | A    |
| 57  | x     | 74   | A    |
| 57  | x     | 76   | C    |

All (32) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 51  | G    |
| 1   | A     | 242 | G    |
| 1   | A     | 372 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 479  | A    |
| 1   | A     | 490  | C    |
| 1   | A     | 710  | U    |
| 1   | A     | 752  | A    |
| 1   | A     | 858  | G    |
| 1   | A     | 859  | G    |
| 1   | A     | 897  | C    |
| 1   | A     | 1020 | A    |
| 1   | A     | 1022 | G    |
| 1   | A     | 1070 | A    |
| 1   | A     | 1111 | A    |
| 1   | A     | 1130 | U    |
| 1   | A     | 1182 | G    |
| 1   | A     | 1190 | G    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1378 | A    |
| 1   | A     | 1399 | C    |
| 1   | A     | 1432 | G    |
| 1   | A     | 1491 | G    |
| 1   | A     | 1940 | U    |
| 1   | A     | 2286 | G    |
| 1   | A     | 2326 | C    |
| 1   | A     | 2333 | A    |
| 1   | A     | 2391 | G    |
| 1   | A     | 2566 | A    |
| 1   | A     | 2655 | G    |
| 1   | A     | 2808 | G    |
| 2   | B     | 66   | A    |
| 2   | B     | 88   | C    |

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is 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$ |
| 59  | GCP  | w     | 601 | -    | 25,34,34     | 2.38 | 7 (28%)     | 31,54,54    | 1.76 | 4 (12%)     |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 59  | GCP  | w     | 601 | -    | -       | 0/18/38/38 | 0/3/3/3 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 59  | w     | 601 | GCP  | C4-N9  | -7.39 | 1.37        | 1.47     |
| 59  | w     | 601 | GCP  | C5-C6  | -4.55 | 1.44        | 1.52     |
| 59  | w     | 601 | GCP  | C8-N9  | -3.20 | 1.37        | 1.46     |
| 59  | w     | 601 | GCP  | C5-C4  | -2.31 | 1.38        | 1.52     |
| 59  | w     | 601 | GCP  | PB-O2B | -2.14 | 1.51        | 1.56     |
| 59  | w     | 601 | GCP  | C6-N1  | 3.02  | 1.38        | 1.33     |
| 59  | w     | 601 | GCP  | PB-O3A | 5.53  | 1.64        | 1.58     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 59  | w     | 601 | GCP  | C5-C6-N1  | -5.35 | 111.90      | 118.27   |
| 59  | w     | 601 | GCP  | PA-O3A-PB | -2.48 | 124.35      | 132.42   |
| 59  | w     | 601 | GCP  | O6-C6-C5  | 3.72  | 127.50      | 119.82   |
| 59  | w     | 601 | GCP  | C4-C5-N7  | 6.11  | 110.56      | 102.46   |

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.