



## Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 05:46 PM UTC

PDB ID : 8Y5R / pdb\_00008y5r  
EMDB ID : EMD-38947  
Title : E.coli Transcription translation coupling complex in TTC-B state 5 (subclass 1) containing mRNA with 27-mer spacer, NusG, NusA, fMet-tRNA(iMet), Phe-tRNA(Phe), and fusidic acid  
Authors : Zhang, J.; Lu, G.; Wang, C.; Lin, J.  
Deposited on : 2024-01-31  
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

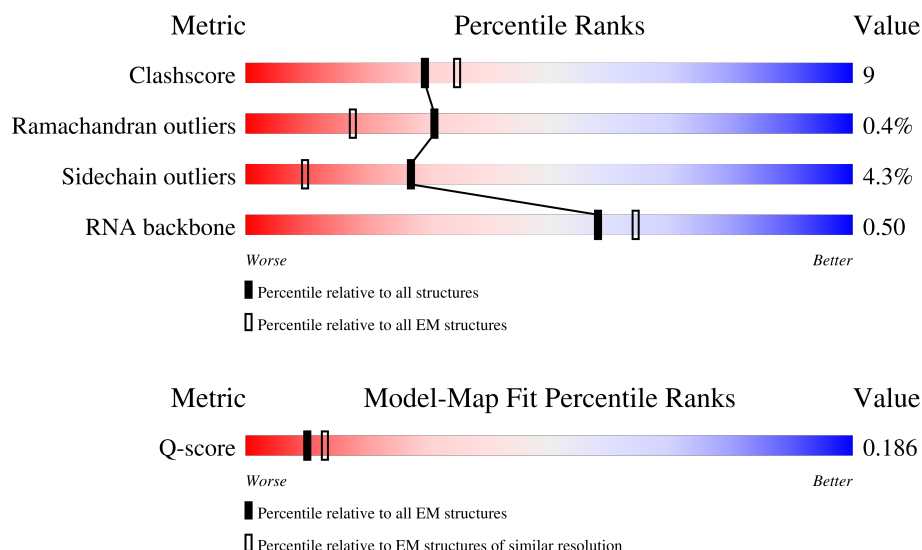
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.50 Å.

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



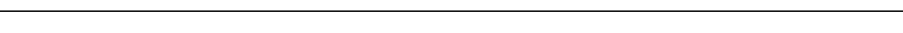
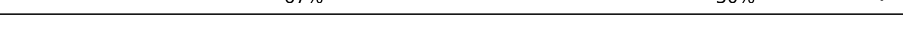
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 2937 ( 4.00 - 5.00 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 70     |                  |
| 2   | B     | 57     |                  |
| 3   | C     | 55     |                  |

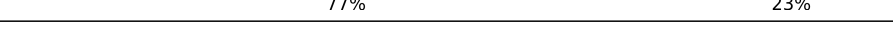
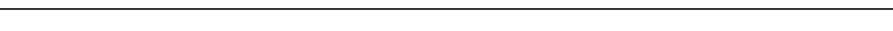
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | D     | 46     |    |
| 5   | E     | 65     |    |
| 6   | F     | 38     |    |
| 7   | G     | 241    |    |
| 8   | H     | 233    |    |
| 9   | I     | 206    |    |
| 10  | J     | 167    |    |
| 11  | K     | 135    |    |
| 12  | L     | 179    |    |
| 13  | M     | 130    |    |
| 14  | N     | 130    |    |
| 15  | O     | 103    |    |
| 16  | P     | 129    |  |
| 17  | Q     | 124    |  |
| 18  | R     | 118    |  |
| 19  | S     | 101    |  |
| 20  | T     | 89     |  |
| 21  | U     | 82     |  |
| 22  | V     | 84     |  |
| 23  | W     | 75     |  |
| 24  | X     | 92     |  |
| 25  | Y     | 87     |  |
| 26  | Z     | 71     |  |
| 27  | b     | 273    |  |
| 28  | c     | 209    |  |

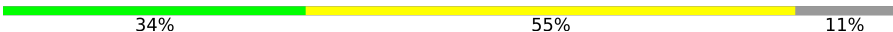
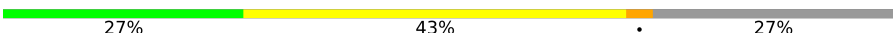
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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 29  | d     | 201    |  81% 19%       |
| 30  | e     | 179    |  78% 21% ..    |
| 31  | f     | 177    |  71% 28% ..    |
| 32  | g     | 149    |  26% 9% 65%    |
| 33  | i     | 142    |  61% 37% ...   |
| 34  | j     | 142    |  85% 15%       |
| 35  | k     | 123    |  79% 20% .     |
| 36  | l     | 144    |  86% 13% .     |
| 37  | m     | 136    |  83% 17%       |
| 38  | n     | 127    |  75% 20% 6%    |
| 39  | o     | 117    |  81% 18% .     |
| 40  | p     | 115    |  86% 12% ..   |
| 41  | q     | 118    |  83% 15% ..  |
| 42  | r     | 103    |  77% 23%     |
| 43  | s     | 110    |  85% 15%     |
| 44  | t     | 100    |  76% 17% 7%  |
| 45  | u     | 104    |  72% 26% .   |
| 46  | v     | 94     |  85% 15%     |
| 47  | w     | 85     |  73% 15% 12% |
| 48  | x     | 78     |  77% 21% ..  |
| 49  | y     | 63     |  78% 22%     |
| 50  | z     | 59     |  76% 22% .   |
| 51  | 1     | 2904   |  43% 51% 7%  |
| 52  | 2     | 120    |  76% 20% .   |
| 53  | 3     | 1542   |  69% 29% .   |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 54  | 4     | 44     |    |
| 55  | 8     | 37     |    |
| 56  | 9     | 37     |    |
| 57  | A1    | 329    |    |
| 57  | A2    | 329    |    |
| 58  | B1    | 1407   |    |
| 59  | B2    | 1342   |    |
| 60  | W0    | 91     |    |
| 61  | NA    | 495    |    |
| 62  | NG    | 181    |    |
| 63  | 5     | 76     |    |
| 64  | 6     | 77     |    |
| 65  | 0     | 716    |  |

## 2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 181797 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | A     | 66       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 521   | 323 | 98 | 94 | 6 |         |       |

- Molecule 2 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | B     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 3   | C     | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 263 | 75 | 71 |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 4   | D     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 5   | E     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | F     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S2.

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

- Molecule 8 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | H     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | I     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | J     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1156  | 719 | 218 | 213 | 6 |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S6, fully modified isoform.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 817   | 515 | 148 | 148 | 6 |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | L     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1181  | 735 | 227 | 215 | 4 |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | M     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | N     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | O     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | P     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 869   | 535 | 173 | 158 | 3 |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | Q     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | R     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 883   | 546 | 178 | 156 | 3 |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | S     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | T     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S16.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | U     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 22 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | V     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |       |

- Molecule 23 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 23  | W     | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 535   | 339 | 100 | 95 | 1 |         |       |

- Molecule 24 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | X     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 637   | 408 | 120 | 107 | 2 |         |       |

- Molecule 25 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Y     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |       |

- Molecule 26 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 26  | Z     | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 544   | 335 | 117 | 91 | 1 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | b     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | c     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | d     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | e     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | f     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32  | g     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 400   | 256 | 73 | 70 | 1 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | i     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | j     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | k     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 938   | 587 | 180 | 165 | 6 |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | l     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | m     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | n     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 39  | o     | 116      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | p     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 41  | q     | 117      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | r     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | s     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | t     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 45  | u     | 102      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |  |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | v     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | w     | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 575   | 356 | 116 | 102 | 1 |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | x     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49  | y     | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 50  | z     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 51 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 51  | 1     | 2903     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62317 | 27801 | 11468 | 20146 | 2902 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference     |
|-------|---------|----------|--------|----------|---------------|
| 1     | 747     | C        | U      | conflict | GB 1929590828 |

- Molecule 52 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 52  | 2     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2568  | 1145 | 471 | 833 | 119 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference    |
|-------|---------|----------|--------|----------|--------------|
| 2     | 120     | A        | U      | conflict | GB NR_103249 |

- Molecule 53 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 53  | 3     | 1539     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33012 | 14725 | 6052 | 10697 | 1538 |         |       |

- Molecule 54 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 54  | 4     | 39       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 809   | 362 | 113 | 295 | 39 |         |       |

- Molecule 55 is a DNA chain called template DNA strand.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 55  | 8     | 27       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 539   | 257 | 88 | 167 | 27 |         |       |

- Molecule 56 is a DNA chain called non-template DNA strand.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 56  | 9     | 20       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 417   | 195 | 84 | 118 | 20 |         |       |

- Molecule 57 is a protein called DNA-directed RNA polymerase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 57  | A1    | 301      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2088  | 1293 | 380 | 409 | 6 |         |       |
| 57  | A2    | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2029  | 1257 | 366 | 400 | 6 |         |       |

- Molecule 58 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 58  | B1    | 1335     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10353 | 6509 | 1842 | 1955 | 47 |         |       |

- Molecule 59 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 59  | B2    | 1340     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10546 | 6616 | 1839 | 2048 | 43 |         |       |

- Molecule 60 is a protein called DNA-directed RNA polymerase subunit omega.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | W0    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 650   | 396 | 122 | 131 | 1 |         |       |

- Molecule 61 is a protein called Transcription termination/antitermination protein NusA.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 61  | NA    | 492      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2432  | 1448 | 492 | 492 |         |       |

- Molecule 62 is a protein called Transcription termination/antitermination protein NusG.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 62  | NG    | 154      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 758   | 450 | 154 | 154 |         |       |

- Molecule 63 is a RNA chain called tRNA(Phe).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 63  | 5     | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1622  | 723 | 290 | 533 | 76 |         |       |

- Molecule 64 is a RNA chain called tRNA(fMet).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 64  | 6     | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |       |

- Molecule 65 is a protein called Elongation factor G.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 65  | 0     | 673      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5211  | 3289 | 900 | 999 | 23 |         |       |

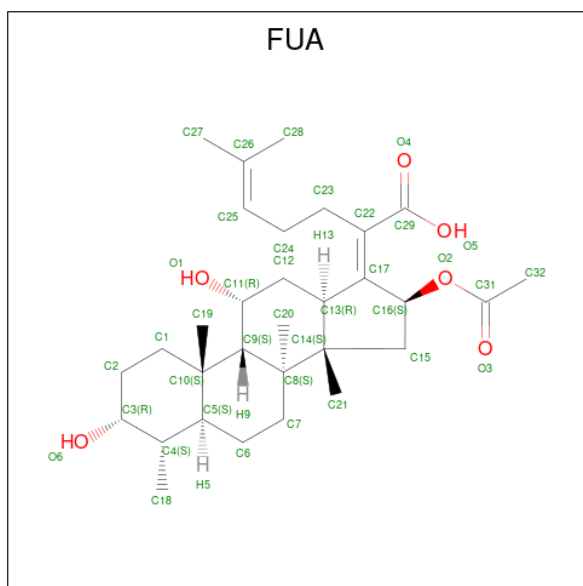
There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| 0     | 705     | GLY      | -      | expression tag | UNP P0A6M8 |
| 0     | 706     | SER      | -      | expression tag | UNP P0A6M8 |
| 0     | 707     | SER      | -      | expression tag | UNP P0A6M8 |
| 0     | 708     | GLY      | -      | expression tag | UNP P0A6M8 |
| 0     | 709     | HIS      | -      | expression tag | UNP P0A6M8 |
| 0     | 710     | HIS      | -      | expression tag | UNP P0A6M8 |
| 0     | 711     | HIS      | -      | expression tag | UNP P0A6M8 |
| 0     | 712     | HIS      | -      | expression tag | UNP P0A6M8 |
| 0     | 713     | HIS      | -      | expression tag | UNP P0A6M8 |
| 0     | 714     | HIS      | -      | expression tag | UNP P0A6M8 |
| 0     | 715     | HIS      | -      | expression tag | UNP P0A6M8 |
| 0     | 716     | HIS      | -      | expression tag | UNP P0A6M8 |

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

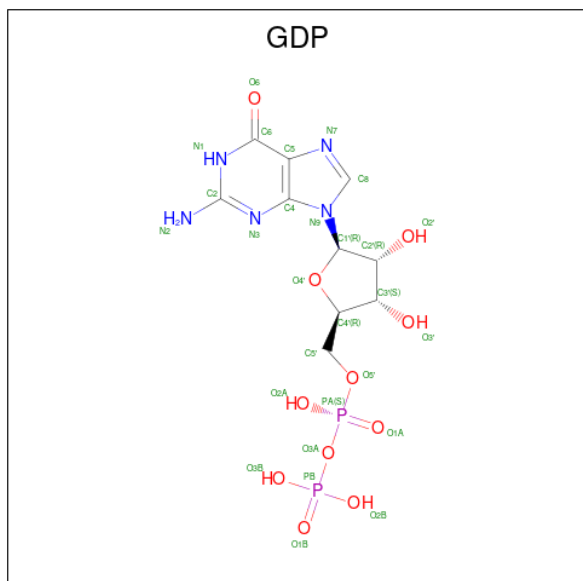
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 66  | B1    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 67 is FUSIDIC ACID (CCD ID: FUA) (formula:  $C_{31}H_{48}O_6$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 67  | 0     | 1        | Total | C  | O | 0       |
|     |       |          | 37    | 31 | 6 |         |

- Molecule 68 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ) (labeled as "Ligand of Interest" by depositor).





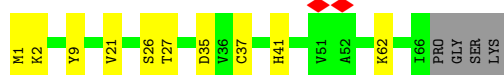
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
|     |       |          | Total | C  | N | O  | P |         |
| 68  | 0     | 1        | 28    | 10 | 5 | 11 | 2 | 0       |

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

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

- Molecule 1: 50S ribosomal protein L31

Chain A: 



- Molecule 2: 50S ribosomal protein L32

Chain B: 



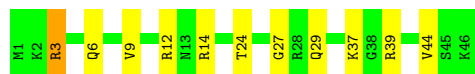
- Molecule 3: 50S ribosomal protein L33

Chain C: 



- Molecule 4: 50S ribosomal protein L34

Chain D: 



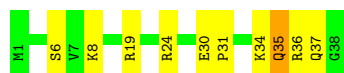
- Molecule 5: 50S ribosomal protein L35

Chain E: 



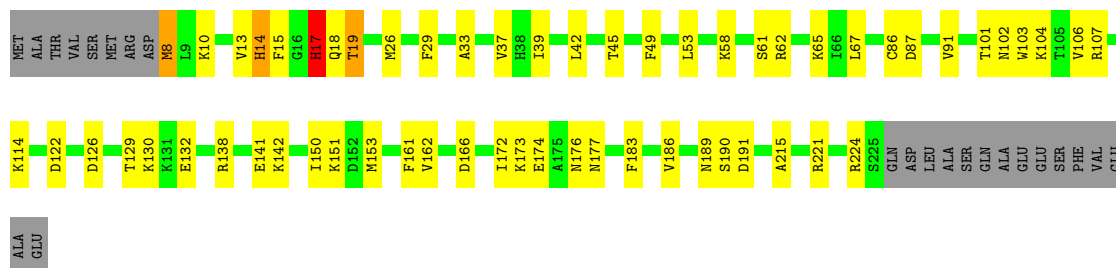
- Molecule 6: 50S ribosomal protein L36

Chain F:  74% 24% .



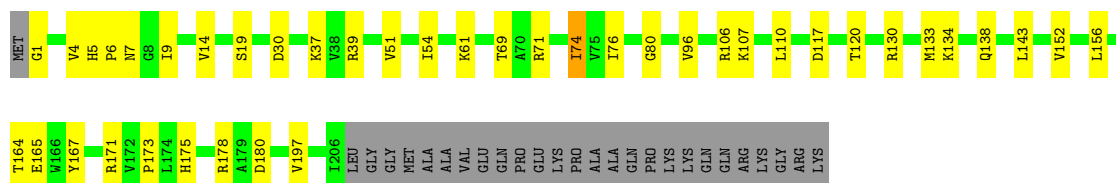
- Molecule 7: 30S ribosomal protein S2

Chain G:  66% 23% . 10%



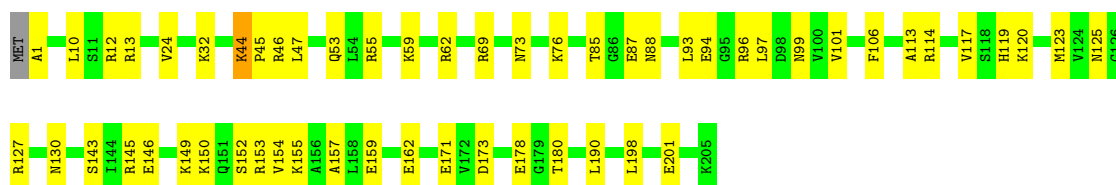
- Molecule 8: 30S ribosomal protein S3

Chain H:  71% 17% 12%



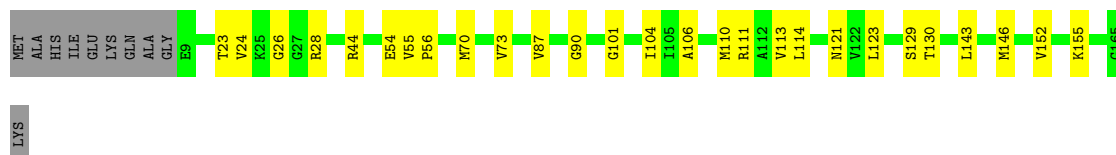
- Molecule 9: 30S ribosomal protein S4

Chain I:  73% 26%



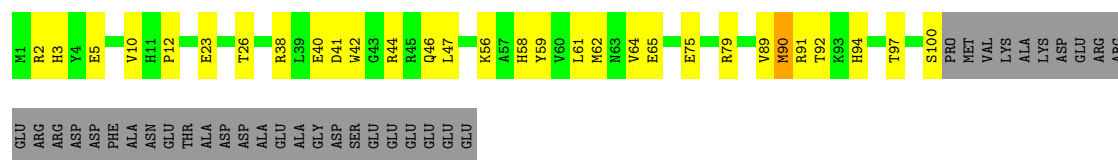
- Molecule 10: 30S ribosomal protein S5

Chain J:  78% 16% 6%



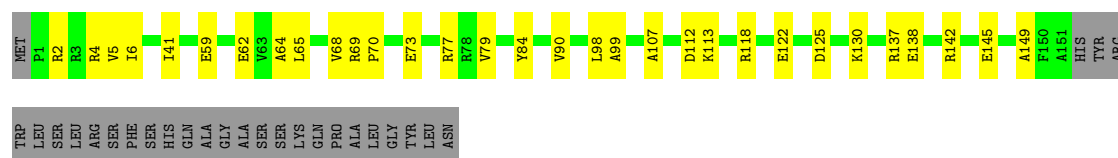
- Molecule 11: 30S ribosomal protein S6, fully modified isoform

Chain K:  52% 21% 26%



- Molecule 12: 30S ribosomal protein S7

Chain L:  67% 17% 16%



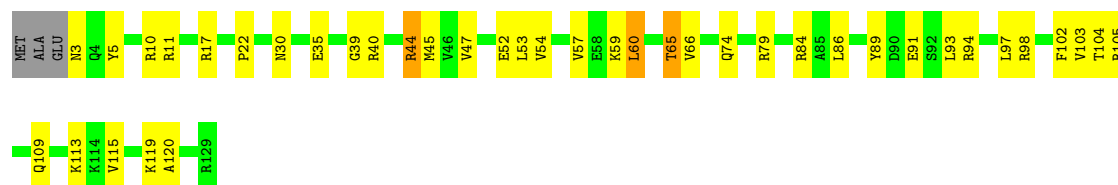
- Molecule 13: 30S ribosomal protein S8

Chain M:  88% 12%



- Molecule 14: 30S ribosomal protein S9

Chain N:  67% 28%



- Molecule 15: 30S ribosomal protein S10

Chain O:  71% 19% 5% 5%



- Molecule 16: 30S ribosomal protein S11

Chain P:  64% 25% 10%





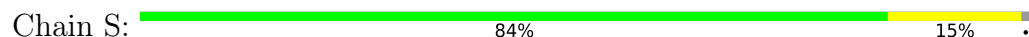
- Molecule 17: 30S ribosomal protein S12



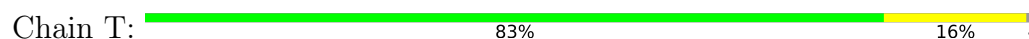
- Molecule 18: 30S ribosomal protein S13



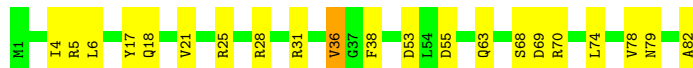
- Molecule 19: 30S ribosomal protein S14



- Molecule 20: 30S ribosomal protein S15



- Molecule 21: 30S ribosomal protein S16



- Molecule 22: 30S ribosomal protein S17





- Molecule 23: 30S ribosomal protein S18

Chain W: 67% 19% 13%



- Molecule 24: 30S ribosomal protein S19

Chain X: 73% 13% 14%



- Molecule 25: 30S ribosomal protein S20

Chain Y: 76% 22%



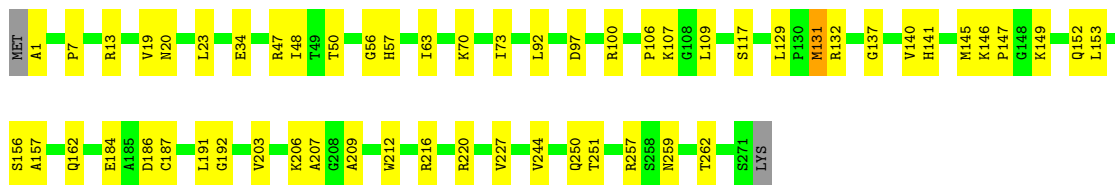
- Molecule 26: 30S ribosomal protein S21

Chain Z: 56% 34% 8%



- Molecule 27: 50S ribosomal protein L2

Chain b: 79% 20%



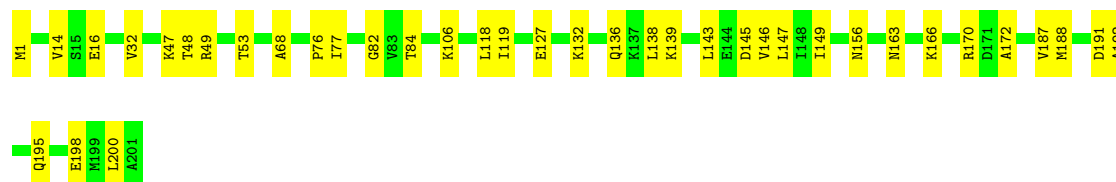
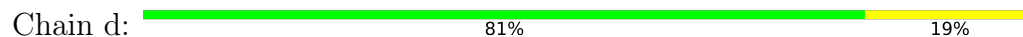
- Molecule 28: 50S ribosomal protein L3

Chain c: 83% 17%

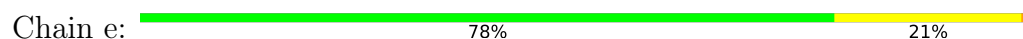




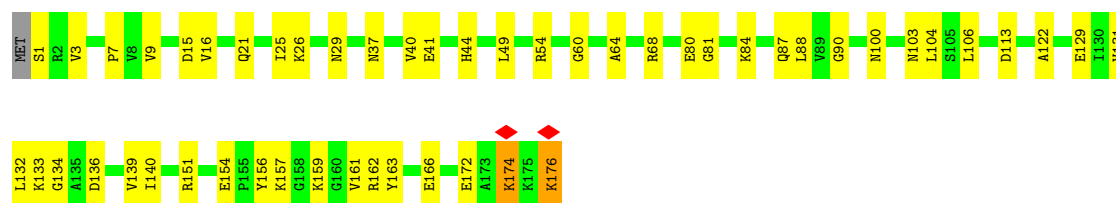
- Molecule 29: 50S ribosomal protein L4



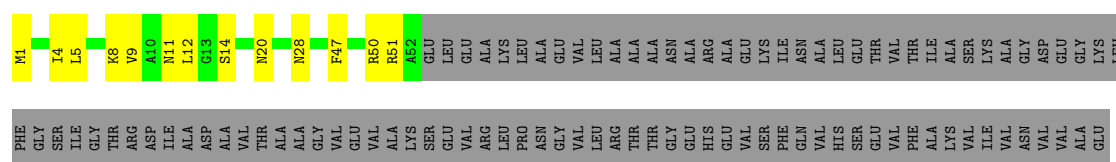
- Molecule 30: 50S ribosomal protein L5



- Molecule 31: 50S ribosomal protein L6

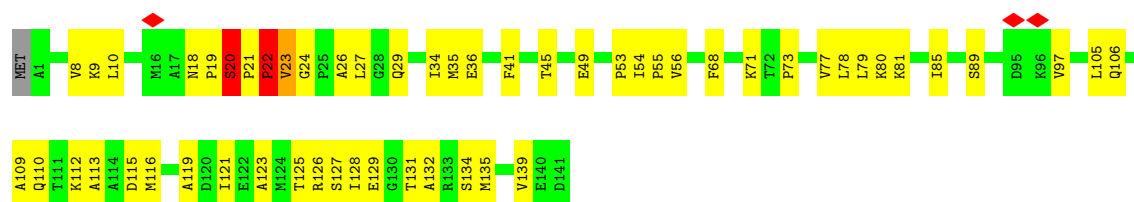


- Molecule 32: 50S ribosomal protein L9



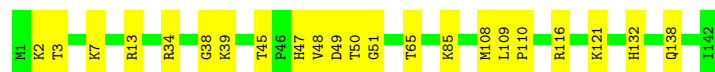
- Molecule 33: 50S ribosomal protein L11





- Molecule 34: 50S ribosomal protein L13

Chain j: 85% 15%



- Molecule 35: 50S ribosomal protein L14

Chain k: 79% 20%



- Molecule 36: 50S ribosomal protein L15

Chain l: 86% 13%



- Molecule 37: 50S ribosomal protein L16

Chain m: 83% 17%



- Molecule 38: 50S ribosomal protein L17

Chain n: 75% 20% 6%



- Molecule 39: 50S ribosomal protein L18

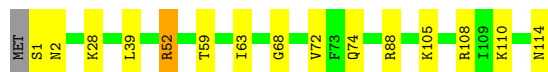
Chain o: 81% 18%



- Molecule 40: 50S ribosomal protein L19



Chain p:  86% 12% ..



- Molecule 41: 50S ribosomal protein L20

Chain q:  83% 15% ..



- Molecule 42: 50S ribosomal protein L21

Chain r:  77% 23%



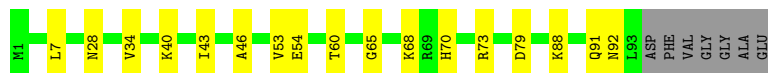
- Molecule 43: 50S ribosomal protein L22

Chain s:  85% 15%



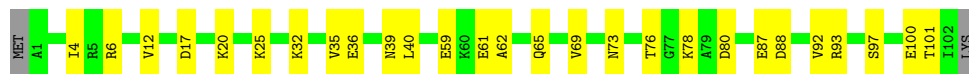
- Molecule 44: 50S ribosomal protein L23

Chain t:  76% 17% 7%



- Molecule 45: 50S ribosomal protein L24

Chain u:  72% 26% .



- Molecule 46: 50S ribosomal protein L25

Chain v:  85% 15%



- Molecule 47: 50S ribosomal protein L27

Chain w:  73% 15% 12%



• Molecule 48: 50S ribosomal protein L28

Chain x:  77% 21% ..



• Molecule 49: 50S ribosomal protein L29

Chain y:  78% 22%



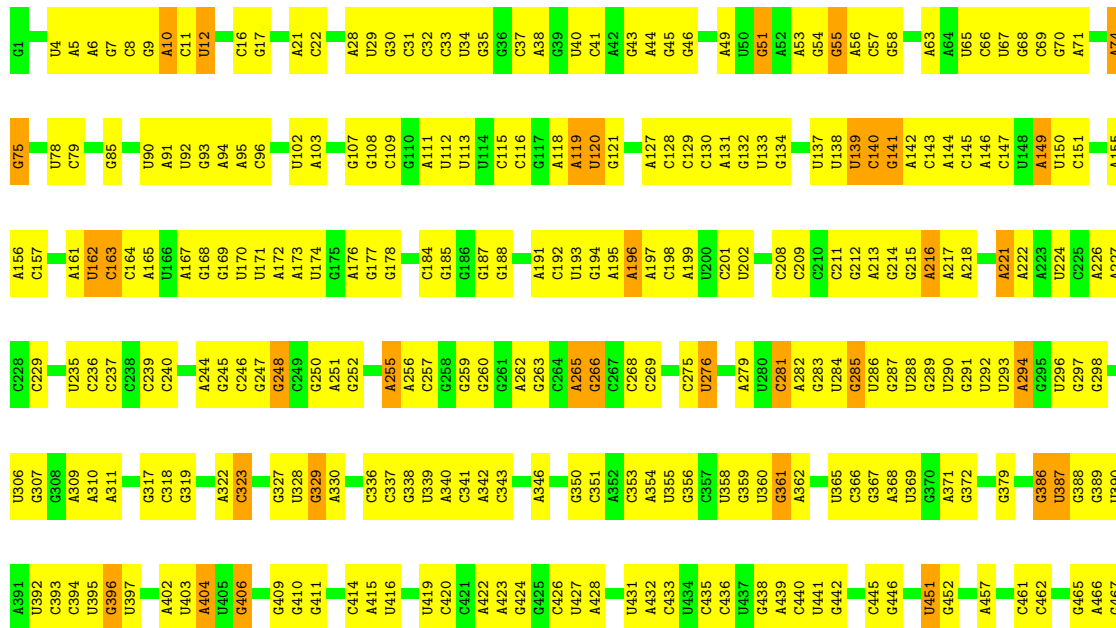
• Molecule 50: 50S ribosomal protein L30

Chain z:  76% 22% .



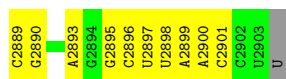
• Molecule 51: 23S rRNA

Chain 1:  43% 51% 7%



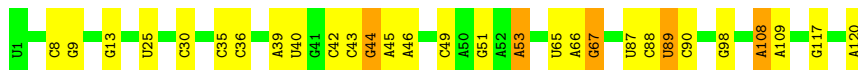
|       |       |       |       |       |       |       |       |      |      |      |      |       |
|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|-------|
| A1572 | U1506 | C1428 | A1336 | U1176 | U1105 | C1043 | C957  | C879 | U709 | A627 | G548 | G468  |
| G1573 | C1507 | G1429 | G1337 | G1177 | G1106 | C1044 | U958  | G805 | G805 | G628 | G549 |       |
| C1574 | A1508 | G1430 | A1338 | C1178 | G1107 | C1045 | A959  | C885 | G712 | G629 | C550 | A472  |
| C1575 | A1509 | G1431 | G1339 | U1179 | U1108 | A1046 | A896  | C889 | G713 | G630 | G551 |       |
|       | G1510 | G1432 |       | U1180 | C1109 | G1047 | C961  | U887 | U810 |      | G552 | G474  |
| U1578 | G1511 | A1433 | G1343 | U1181 | G1110 | A1048 | C968  | C888 | A718 | A633 | G553 |       |
| A1579 | C1512 | A1434 | U1344 | G1182 | A1111 | C1049 |       | C889 | C719 | C634 | U554 | G476  |
|       |       | G1435 | C1345 | U1183 | G1112 | A1050 |       | C890 | C719 | C634 | U554 |       |
| A1515 | A1516 | G1436 | A1346 | U1184 | U1113 |       |       | C891 | U720 | C635 | G555 | A1580 |
| C1581 | G1517 | C1437 | A1347 | U1185 | C1114 | A1054 | A972  | C891 | A721 | G636 | A556 | C1582 |
| C1582 | U1518 | U1438 | C1348 | G1280 | G1115 | G1055 | G974  | C892 | A722 | A637 | C557 | A1583 |
| A1583 | C1517 | A1439 | C1349 | G1281 | G1116 | G1056 | A975  | C893 | C723 | G638 | U558 |       |
|       | U1519 | U1440 |       | U1188 | C1117 | A1057 |       | A819 | U724 | U639 |      |       |
| G1588 | U1520 | G1441 | U1352 | U1282 | C1118 | A1058 | A979  | A820 | G725 | C640 | U562 | G488  |
| U1589 | U1521 | U1442 | U1353 | G1283 | C1119 | U1059 | C897  | A821 | G726 | U641 | A563 | G489  |
| A1590 | A1522 | U1443 | A1365 | A1284 | U1119 | G1060 | A980  |      | A727 |      | C490 | G490  |
| A1591 | U1523 | C1444 | A1366 | U1194 | G1120 | U1061 | A981  | A825 | G728 | A644 | U566 | G492  |
| A1593 | G1524 | G1448 | A1367 | U1195 | C1121 | A1062 | C982  | U826 | G729 | U645 | U567 | G493  |
| U1594 | A1525 | G1449 | G1368 | C1196 |       | G1063 | A983  | U827 | A730 | U646 | U568 |       |
| C1595 | C1526 | G1450 |       | G1197 | U1130 | G1064 | A984  | U828 |      | G647 | U569 | G494  |
|       | U1527 | C1451 | U1377 | U1198 | G1131 | U1065 | C985  | C901 | C736 | G648 | U570 | G498  |
| A1596 | G1527 | C1452 | A1378 | U1199 | G1132 | U1066 | A829  | C902 | G745 | U571 | U499 | G500  |
| U1597 | A1528 | A1453 | U1379 | C1200 | A1133 | A1067 |       | C903 | U746 | A572 | U572 | G501  |
| A1598 | G1529 | C1454 | G1380 |       | A1134 | A1067 |       | A905 | C747 | A574 | U573 |       |
| U1599 | G1530 |       | U1381 | A1204 | C1135 | G1068 | C993  | U906 |      | U652 | U574 | G499  |
| C1600 |       | C1461 | G1382 | A1205 | G1136 | A1069 | C994  | G907 |      | U653 | A575 | G502  |
| G1601 | C1533 | C1462 | A1383 | U1213 | G1137 | A1070 | C995  | C908 | A752 | A654 | A576 | A503  |
| U1602 | U1534 | G1463 | A1382 | U1209 | G1138 | G1071 | A996  | A909 |      | G656 | U580 | A504  |
| A1603 | A1535 | G1464 | C1383 | G1210 | G1139 | C1072 |       | A910 | G757 |      |      | G506  |
| C1604 | C1536 | G1465 | U1386 | G1299 | G1140 | A1073 | C1005 | A911 |      | G662 | A586 |       |
| G1605 | G1537 | U1466 | A1387 | G1300 | U1141 | G1074 |       | C840 | G759 |      | C510 |       |
| C1606 | U1538 | U1467 | G1388 | A1301 | A1142 | C1075 | A1009 | G914 | G760 | G669 | A590 | U511  |
| C1607 | U1539 | U1468 | G1389 | A1302 | A1143 | G1076 | A1010 | C915 | A761 | U670 | U591 |       |
| A1608 | G1540 | A1469 | U1390 | A1306 | A1144 | U1077 | G1011 |      | U762 | C671 | G518 |       |
|       | U1542 | U1394 |       |       | C1145 | U1078 | A918  | A845 | G763 | C672 | U519 |       |
| A1614 | U1543 |       |       |       | C1146 | C1079 | U919  | U846 | A764 | C673 | G520 |       |
| C1615 | A1544 | U1400 |       | G1225 | A1147 | A1080 | A1014 | U847 | C765 | G674 | C595 | U521  |
| A1616 | C1545 | U1401 | U1400 | G1226 | U1148 | U1081 | U1015 |      |      |      | U596 | A522  |
|       | U1546 | G1482 | G1401 | A1230 | G1149 | U1082 |       | G923 | G774 | A677 | G597 |       |
| C1625 | G1546 | G1483 | U1402 | U1231 | C1150 | A1083 | U1019 | G924 | G775 | C678 | U598 |       |
| A1626 |       | U1484 | A1403 | G1232 | A1151 | A1084 | C679  | A926 | U779 | C679 | A599 |       |
|       | C1550 | U1485 | C1404 | C1233 | C1152 | A1085 | A1021 | U852 | C680 | C680 | A603 | C527  |
| A1634 | A1551 | U1486 | U1405 | C1234 | C1153 | A1086 | G1022 | U853 | G780 | G681 |      | A528  |
|       | A1552 | U1487 | U1406 | A1237 | G1154 | G1087 | U1023 | C853 | C781 | G682 | A603 | A529  |
| G1642 | A1553 | C1488 |       | G1238 | A1155 | A1088 | G1024 | C854 | A782 | U683 | U607 | G530  |
| G1643 | U1554 | C1489 | U1409 | G1239 | A1156 | A1089 | G1025 | C855 | G783 | A684 | A608 | A532  |
| C1644 | G1555 | C1490 | U1410 | U1240 | G1157 | A1090 | A1026 |      | U784 | G685 | A609 | G533  |
| G1645 |       | G1491 | U1411 | A1321 |       | G1091 | A1027 | C935 | G785 | U686 | C610 | U534  |
| U1646 | C1558 | G1492 | U1412 | A1322 | G1160 | C1092 |       | A936 |      | C687 | C611 | G535  |
| U1647 | U1559 | C1493 | A1413 | G1323 | C1161 | G1093 | G1031 | C937 | A788 | U688 | G612 | G536  |
| U1648 | G1560 | C1414 | U1415 | G1324 | G1162 | U1094 | A1032 | C938 | A789 | A613 | G537 |       |
|       | A1561 | A1495 | C1415 | U1325 | G1163 | A1095 | U1033 | C939 | U790 | A614 | G538 |       |
| U1562 |       | U1496 | G1416 | U1326 | C1164 | A1096 | G1034 | C791 | G696 | U615 | G539 |       |
|       |       | U1497 | C1417 | A1327 | A1165 | U1097 | U1035 | A941 | A792 | A616 | C540 |       |
|       |       |       | G1418 | A1328 | G1256 | A1098 | G1036 | C942 | U793 | G697 | A541 |       |
|       | C1563 |       |       | U1329 | C1257 | A1099 | G1037 |      | A794 | U703 | G542 |       |
| U1662 | U1566 | G1500 | A1419 | C1330 | G1170 | C1100 | G1038 | C946 | A795 | G704 | A621 |       |
| G1663 | U1567 | G1501 | A1420 | U1331 | G1171 | U1101 | A1039 | A947 | C796 | A705 | G622 | C544  |
|       |       | A1502 |       | G1333 | U1172 | C1102 | A1040 |      |      | A706 | G623 |       |
| G1666 | U1568 | A1503 | G1425 | G1334 | U1173 | C1102 | A1040 |      |      | A707 | C624 |       |
| C1667 | A1569 | A1504 | G1426 | C1335 | U1174 | A1103 | G1041 | U955 | A800 | G707 | U546 |       |
| A1668 | U1570 | A1505 | A1427 | G1336 | A1175 | C1104 | C1042 | C956 | A877 |      | A547 |       |
| A1669 | A1571 | A1506 | A1428 | C1337 | U1176 | C1105 |       |      |      |      |      |       |





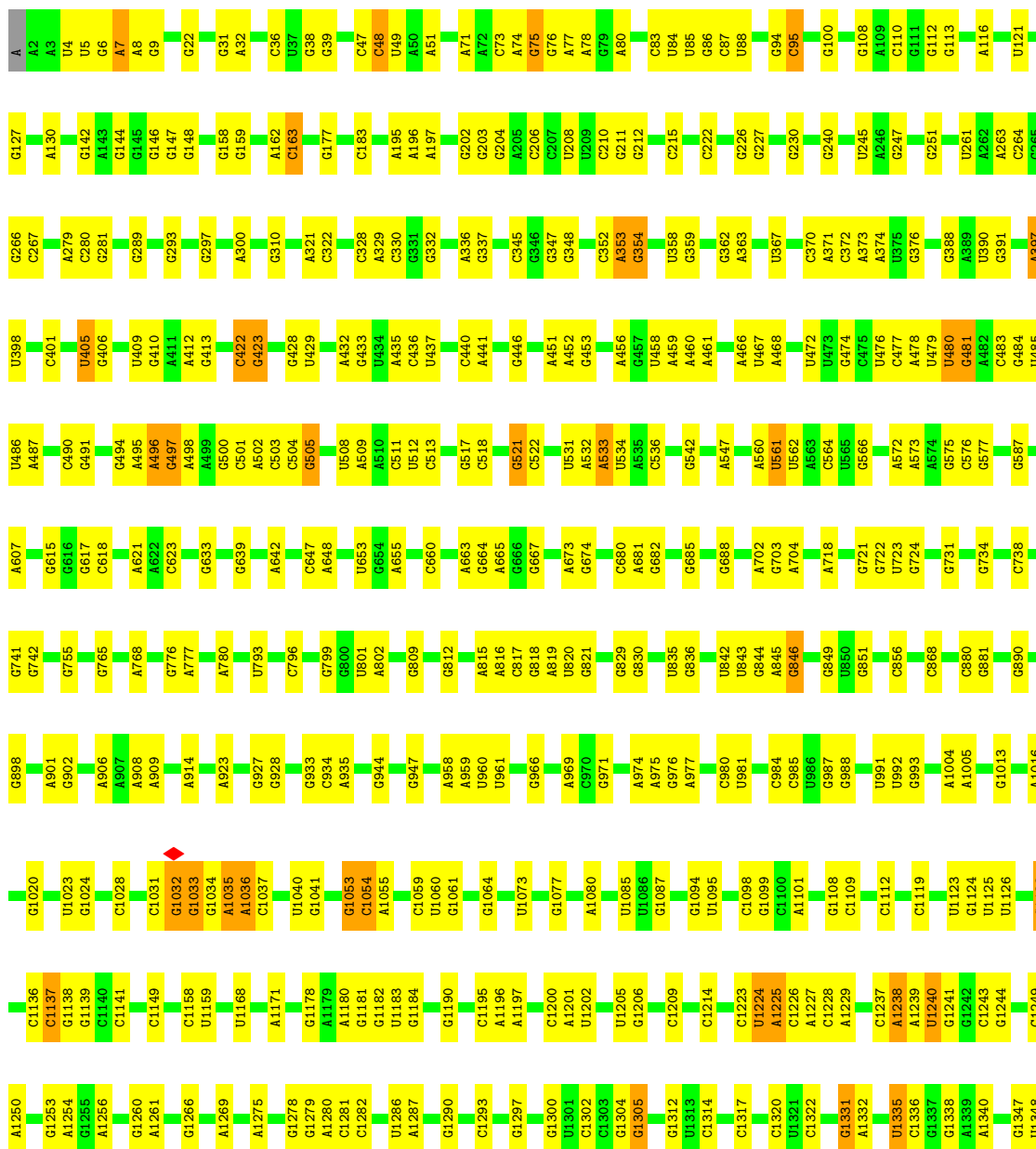
• Molecule 52: 5S rRNA

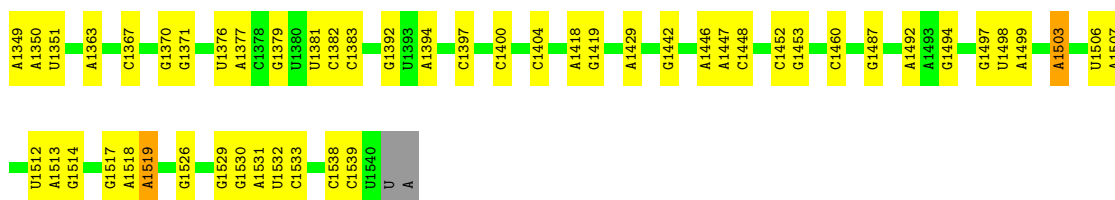
Chain 2: 76% 20% .



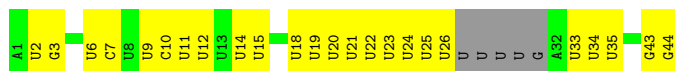
• Molecule 53: 16S rRNA

Chain 3: 69% 29% .

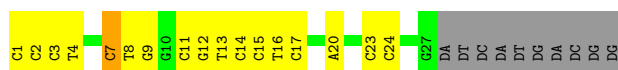




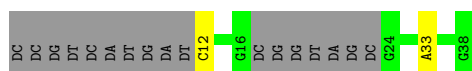
- Molecule 54: mRNA



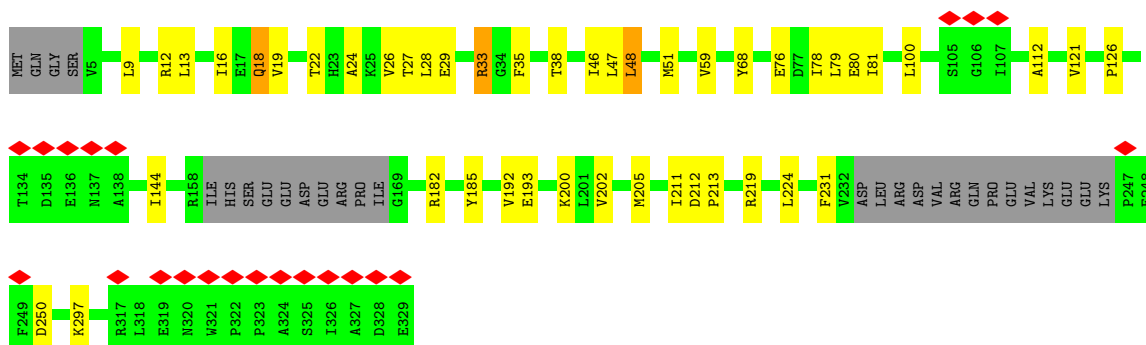
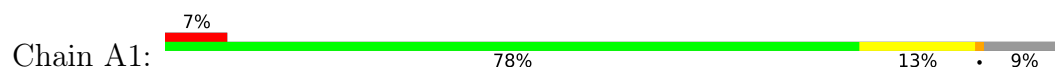
- Molecule 55: template DNA strand



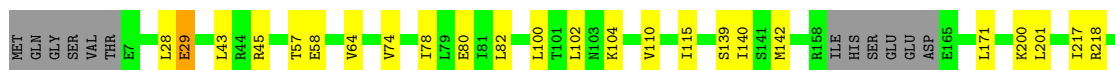
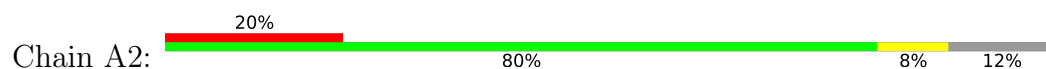
- Molecule 56: non-template DNA strand



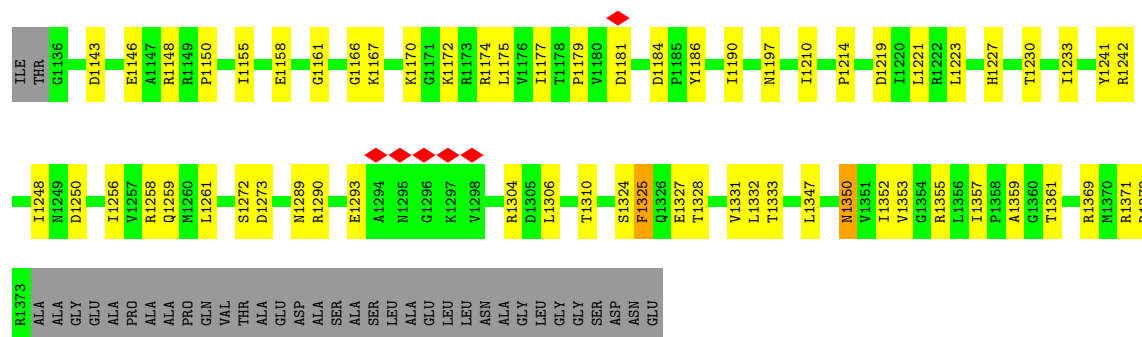
- Molecule 57: DNA-directed RNA polymerase subunit alpha



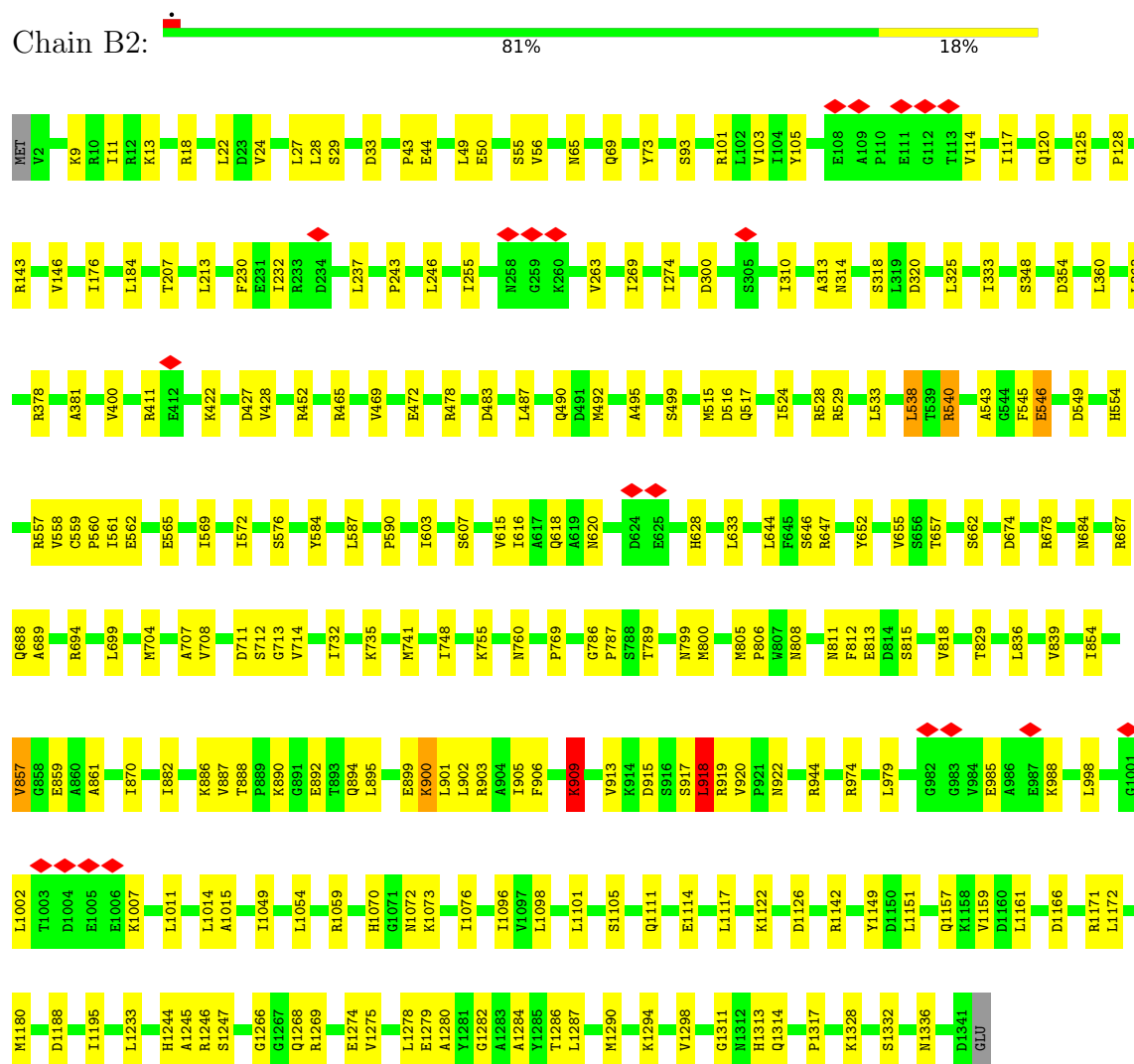
- Molecule 57: DNA-directed RNA polymerase subunit alpha



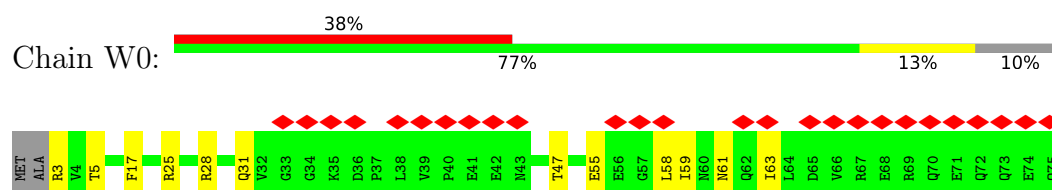




• Molecule 59: DNA-directed RNA polymerase subunit beta



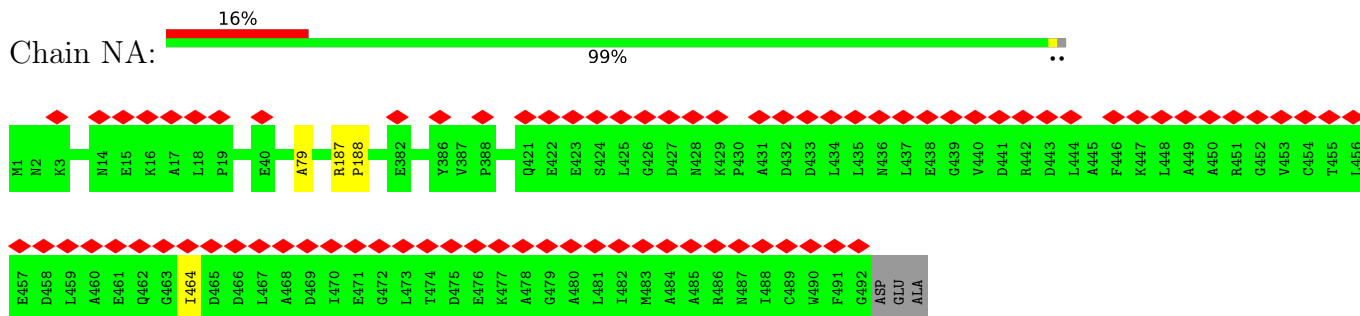
• Molecule 60: DNA-directed RNA polymerase subunit omega



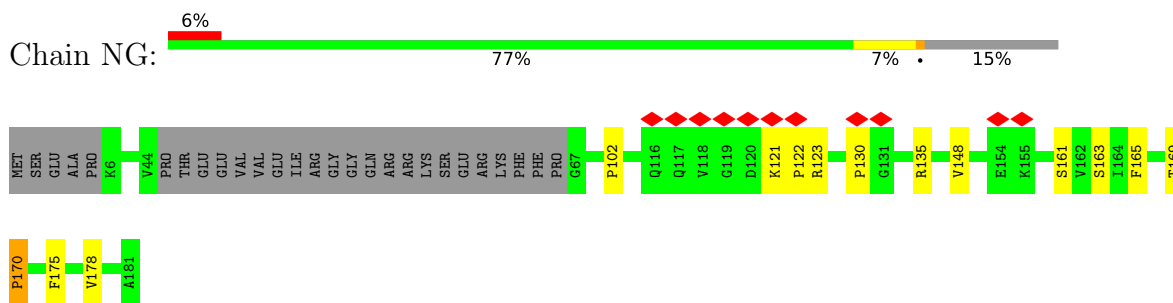


ALA  
GLU  
GLY  
ARG

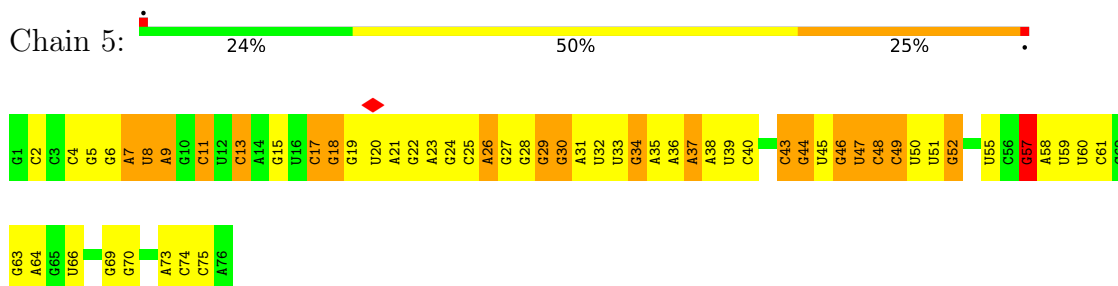
- Molecule 61: Transcription termination/antitermination protein NusA



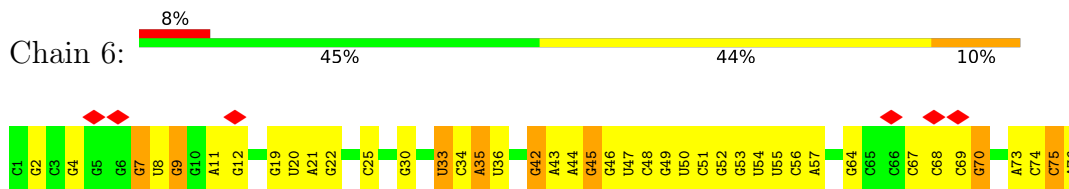
- Molecule 62: Transcription termination/antitermination protein NusG



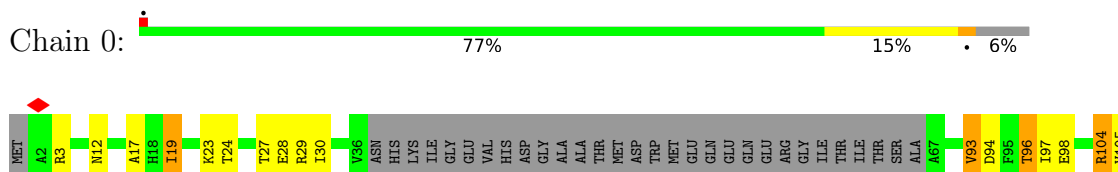
- Molecule 63: tRNA(Phe)

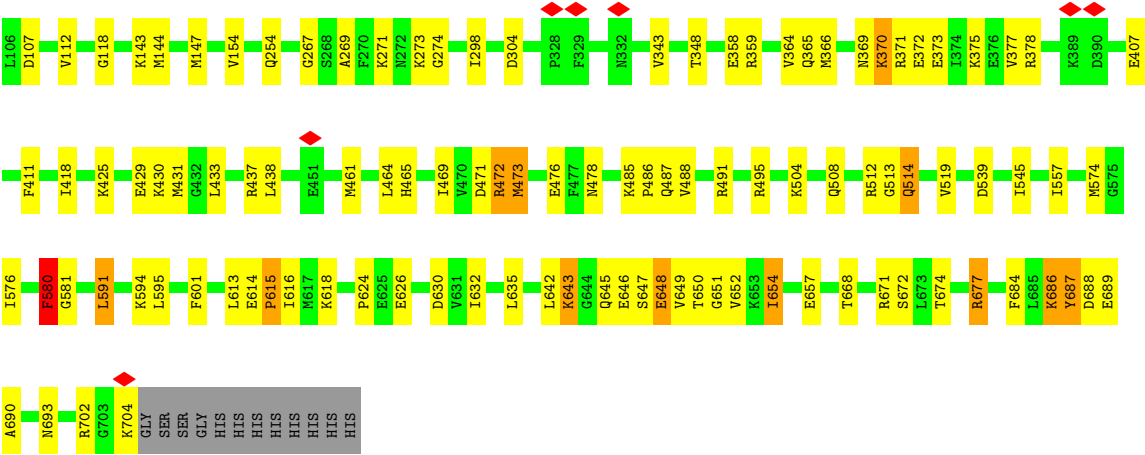


- Molecule 64: tRNA(fMet)



- Molecule 65: Elongation factor G





## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, Not provided             |           |
| Number of particles used             | 609587                          | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | NONE                            | Depositor |
| Microscope                           | FEI TALOS ARCTICA               | Depositor |
| Voltage (kV)                         | 200                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 47                              | Depositor |
| Minimum defocus (nm)                 | 500                             | Depositor |
| Maximum defocus (nm)                 | 1500                            | Depositor |
| Magnification                        | Not provided                    |           |
| Image detector                       | FEI FALCON III (4k x 4k)        | Depositor |
| Maximum map value                    | 0.087                           | Depositor |
| Minimum map value                    | -0.033                          | Depositor |
| Average map value                    | 0.000                           | Depositor |
| Map value standard deviation         | 0.004                           | Depositor |
| Recommended contour level            | 0.007                           | Depositor |
| Map size ( $\text{\AA}$ )            | 753.60004, 753.60004, 753.60004 | wwPDB     |
| Map dimensions                       | 480, 480, 480                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.57, 1.57, 1.57                | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$   |
| 1   | A     | 0.26         | 0/530       | 0.54        | 0/707         |
| 2   | B     | 0.40         | 0/450       | 0.60        | 0/599         |
| 3   | C     | 0.27         | 0/416       | 0.52        | 0/554         |
| 4   | D     | 0.47         | 0/380       | 0.76        | 2/498 (0.4%)  |
| 5   | E     | 0.53         | 0/513       | 0.60        | 0/676         |
| 6   | F     | 0.58         | 0/303       | 0.66        | 0/397         |
| 7   | G     | 0.37         | 0/1735      | 0.64        | 0/2338        |
| 8   | H     | 0.34         | 0/1651      | 0.55        | 0/2225        |
| 9   | I     | 0.35         | 0/1665      | 0.71        | 0/2227        |
| 10  | J     | 0.38         | 0/1169      | 0.68        | 2/1573 (0.1%) |
| 11  | K     | 0.46         | 0/835       | 0.77        | 0/1128        |
| 12  | L     | 0.30         | 0/1195      | 0.66        | 3/1602 (0.2%) |
| 13  | M     | 0.35         | 0/989       | 0.52        | 0/1326        |
| 14  | N     | 0.47         | 0/1034      | 0.77        | 0/1375        |
| 15  | O     | 0.50         | 0/796       | 0.78        | 2/1077 (0.2%) |
| 16  | P     | 0.45         | 0/885       | 0.64        | 1/1195 (0.1%) |
| 17  | Q     | 0.50         | 0/969       | 0.86        | 2/1300 (0.2%) |
| 18  | R     | 0.33         | 0/892       | 0.73        | 2/1193 (0.2%) |
| 19  | S     | 0.33         | 0/817       | 0.61        | 0/1088        |
| 20  | T     | 0.49         | 0/722       | 0.64        | 0/964         |
| 21  | U     | 0.30         | 0/659       | 0.71        | 2/884 (0.2%)  |
| 22  | V     | 0.44         | 0/657       | 0.71        | 0/881         |
| 23  | W     | 0.54         | 0/544       | 0.74        | 1/731 (0.1%)  |
| 24  | X     | 0.28         | 0/652       | 0.55        | 0/877         |
| 25  | Y     | 0.28         | 0/671       | 0.52        | 0/888         |
| 26  | Z     | 0.66         | 0/550       | 1.01        | 2/728 (0.3%)  |
| 27  | b     | 0.49         | 0/2121      | 0.64        | 0/2852        |
| 28  | c     | 0.42         | 0/1586      | 0.59        | 2/2134 (0.1%) |
| 29  | d     | 0.43         | 0/1571      | 0.62        | 0/2113        |
| 30  | e     | 0.43         | 0/1434      | 0.65        | 2/1926 (0.1%) |
| 31  | f     | 0.35         | 0/1343      | 0.55        | 0/1816        |
| 32  | g     | 0.32         | 0/405       | 0.75        | 0/544         |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 33  | i     | 0.51         | 0/1046          | 0.87        | 3/1410 (0.2%)    |
| 34  | j     | 0.41         | 0/1152          | 0.55        | 1/1551 (0.1%)    |
| 35  | k     | 0.45         | 0/947           | 0.66        | 0/1268           |
| 36  | l     | 0.40         | 0/1054          | 0.63        | 0/1403           |
| 37  | m     | 0.56         | 0/1093          | 0.74        | 0/1460           |
| 38  | n     | 0.46         | 0/973           | 0.72        | 1/1301 (0.1%)    |
| 39  | o     | 0.32         | 0/902           | 0.51        | 0/1209           |
| 40  | p     | 0.42         | 0/929           | 0.63        | 0/1242           |
| 41  | q     | 0.52         | 0/960           | 0.62        | 1/1278 (0.1%)    |
| 42  | r     | 0.45         | 0/829           | 0.69        | 0/1107           |
| 43  | s     | 0.43         | 0/864           | 0.58        | 0/1156           |
| 44  | t     | 0.33         | 0/744           | 0.52        | 0/994            |
| 45  | u     | 0.46         | 0/787           | 0.75        | 0/1051           |
| 46  | v     | 0.34         | 0/766           | 0.51        | 0/1025           |
| 47  | w     | 0.40         | 0/582           | 0.52        | 0/769            |
| 48  | x     | 0.43         | 0/635           | 0.63        | 1/848 (0.1%)     |
| 49  | y     | 0.29         | 0/510           | 0.64        | 0/677            |
| 50  | z     | 0.41         | 0/453           | 0.53        | 0/605            |
| 51  | 1     | 0.51         | 0/69796         | 0.62        | 21/108888 (0.0%) |
| 52  | 2     | 0.43         | 0/2872          | 0.46        | 0/4479           |
| 53  | 3     | 0.42         | 0/36963         | 0.43        | 0/57662          |
| 54  | 4     | 0.52         | 0/896           | 0.68        | 0/1387           |
| 55  | 8     | 0.56         | 0/599           | 0.71        | 1/919 (0.1%)     |
| 56  | 9     | 0.49         | 0/468           | 0.53        | 0/719            |
| 57  | A1    | 0.55         | 0/2106          | 0.81        | 0/2868           |
| 57  | A2    | 0.49         | 0/2048          | 0.76        | 0/2786           |
| 58  | B1    | 0.57         | 4/10510 (0.0%)  | 0.75        | 8/14196 (0.1%)   |
| 59  | B2    | 0.46         | 0/10714         | 0.67        | 0/14459          |
| 60  | W0    | 0.30         | 0/652           | 0.60        | 0/879            |
| 61  | NA    | 0.78         | 0/2431          | 1.22        | 0/3385           |
| 62  | NG    | 1.12         | 0/756           | 1.07        | 0/1048           |
| 63  | 5     | 0.57         | 0/1812          | 0.85        | 1/2823 (0.0%)    |
| 64  | 6     | 0.39         | 0/1832          | 0.57        | 1/2855 (0.0%)    |
| 65  | 0     | 0.84         | 0/5308          | 1.17        | 6/7181 (0.1%)    |
| All | All   | 0.49         | 4/195128 (0.0%) | 0.64        | 68/287304 (0.0%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 58  | B1    | 1350 | ASN  | CG-ND2 | -5.28 | 1.22        | 1.33     |
| 58  | B1    | 1108 | GLN  | CD-OE1 | 5.18  | 1.33        | 1.23     |
| 58  | B1    | 424  | ASN  | CG-ND2 | -5.13 | 1.22        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 58  | B1    | 665 | GLN  | CD-OE1 | 5.04 | 1.33        | 1.23     |

All (68) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 65  | 0     | 580  | PHE  | CA-CB-CG    | 9.59  | 123.39      | 113.80   |
| 16  | P     | 73   | VAL  | N-CA-C      | -9.05 | 104.52      | 113.20   |
| 41  | q     | 33   | VAL  | N-CA-C      | -8.73 | 104.78      | 112.12   |
| 12  | L     | 64   | ALA  | N-CA-C      | -7.68 | 105.07      | 114.75   |
| 51  | 1     | 1130 | U    | C2'-C3'-O3' | 7.63  | 120.94      | 109.50   |
| 64  | 6     | 33   | U    | C2'-C3'-O3' | 7.28  | 120.41      | 109.50   |
| 51  | 1     | 2326 | C    | C2'-C3'-O3' | 7.18  | 120.27      | 109.50   |
| 58  | B1    | 450  | HIS  | CB-CG-CD2   | -6.58 | 122.65      | 131.20   |
| 51  | 1     | 761  | A    | C4'-C3'-O3' | -6.49 | 103.26      | 113.00   |
| 65  | 0     | 615  | PRO  | CB-CA-C     | -6.47 | 102.50      | 110.98   |
| 58  | B1    | 777  | HIS  | CB-CG-CD2   | -6.41 | 122.87      | 131.20   |
| 58  | B1    | 61   | ILE  | CA-C-N      | -6.36 | 114.01      | 121.64   |
| 58  | B1    | 61   | ILE  | C-N-CA      | -6.36 | 114.01      | 121.64   |
| 28  | c     | 147  | GLY  | CA-C-N      | -6.02 | 115.28      | 122.44   |
| 28  | c     | 147  | GLY  | C-N-CA      | -6.02 | 115.28      | 122.44   |
| 58  | B1    | 450  | HIS  | CB-CG-ND1   | 5.69  | 131.23      | 122.70   |
| 51  | 1     | 2060 | A    | C2'-C3'-O3' | 5.68  | 118.03      | 109.50   |
| 65  | 0     | 657  | GLU  | CA-C-N      | -5.63 | 118.43      | 123.33   |
| 65  | 0     | 657  | GLU  | C-N-CA      | -5.63 | 118.43      | 123.33   |
| 26  | Z     | 35   | GLU  | CA-C-N      | 5.60  | 132.23      | 121.54   |
| 26  | Z     | 35   | GLU  | C-N-CA      | 5.60  | 132.23      | 121.54   |
| 51  | 1     | 1790 | C    | N1-C1'-C2'  | 5.60  | 120.39      | 112.00   |
| 15  | O     | 57   | VAL  | CA-C-N      | 5.59  | 132.22      | 121.54   |
| 15  | O     | 57   | VAL  | C-N-CA      | 5.59  | 132.22      | 121.54   |
| 38  | n     | 47   | VAL  | N-CA-C      | -5.56 | 107.45      | 112.12   |
| 10  | J     | 155  | LYS  | N-CA-C      | -5.53 | 107.79      | 114.75   |
| 51  | 1     | 960  | A    | N9-C1'-C2'  | 5.47  | 120.21      | 112.00   |
| 51  | 1     | 1451 | C    | N1-C1'-C2'  | 5.47  | 120.21      | 112.00   |
| 51  | 1     | 1905 | C    | C4'-C3'-O3' | -5.47 | 104.79      | 113.00   |
| 58  | B1    | 777  | HIS  | CB-CG-ND1   | 5.47  | 130.90      | 122.70   |
| 51  | 1     | 1020 | A    | C2'-C3'-O3' | 5.43  | 117.64      | 109.50   |
| 51  | 1     | 1696 | G    | N9-C1'-C2'  | 5.42  | 120.14      | 112.00   |
| 4   | D     | 3    | ARG  | CA-C-N      | 5.40  | 127.78      | 120.38   |
| 4   | D     | 3    | ARG  | C-N-CA      | 5.40  | 127.78      | 120.38   |
| 55  | 8     | 7    | DC   | C2'-C3'-O3' | -5.40 | 103.40      | 111.50   |
| 65  | 0     | 271  | LYS  | N-CA-C      | -5.32 | 106.30      | 112.89   |
| 51  | 1     | 1782 | U    | N1-C1'-C2'  | 5.31  | 119.97      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 51  | 1     | 2428 | G    | N9-C1'-C2'  | 5.29  | 119.93      | 112.00   |
| 30  | e     | 141  | ASP  | CA-C-N      | 5.24  | 131.56      | 121.54   |
| 30  | e     | 141  | ASP  | C-N-CA      | 5.24  | 131.56      | 121.54   |
| 51  | 1     | 2055 | C    | N1-C1'-C2'  | 5.23  | 119.85      | 112.00   |
| 51  | 1     | 980  | A    | N9-C1'-C2'  | 5.23  | 119.84      | 112.00   |
| 12  | L     | 5    | VAL  | CA-C-N      | 5.22  | 127.70      | 120.49   |
| 12  | L     | 5    | VAL  | C-N-CA      | 5.22  | 127.70      | 120.49   |
| 34  | j     | 110  | PRO  | N-CA-C      | 5.22  | 120.72      | 113.98   |
| 51  | 1     | 2576 | G    | N9-C1'-C2'  | 5.21  | 119.82      | 112.00   |
| 58  | B1    | 27   | PRO  | N-CA-C      | -5.21 | 106.26      | 113.81   |
| 21  | U     | 78   | VAL  | CA-C-N      | 5.19  | 129.65      | 121.56   |
| 21  | U     | 78   | VAL  | C-N-CA      | 5.19  | 129.65      | 121.56   |
| 51  | 1     | 2430 | A    | N9-C1'-C2'  | 5.16  | 119.74      | 112.00   |
| 51  | 1     | 1565 | C    | N1-C1'-C2'  | 5.15  | 119.72      | 112.00   |
| 23  | W     | 14   | ALA  | N-CA-C      | -5.14 | 106.09      | 112.93   |
| 51  | 1     | 1328 | A    | N9-C1'-C2'  | 5.14  | 119.71      | 112.00   |
| 18  | R     | 3    | ILE  | CA-C-N      | 5.11  | 131.30      | 121.54   |
| 18  | R     | 3    | ILE  | C-N-CA      | 5.11  | 131.30      | 121.54   |
| 63  | 5     | 57   | G    | C4'-C3'-O3' | 5.11  | 117.06      | 109.40   |
| 33  | i     | 71   | LYS  | CA-C-N      | 5.10  | 134.24      | 121.80   |
| 33  | i     | 71   | LYS  | C-N-CA      | 5.10  | 134.24      | 121.80   |
| 58  | B1    | 61   | ILE  | CA-C-O      | -5.10 | 115.65      | 120.95   |
| 10  | J     | 87   | VAL  | N-CA-C      | 5.09  | 115.97      | 109.30   |
| 65  | 0     | 375  | LYS  | N-CA-C      | -5.09 | 106.92      | 112.72   |
| 33  | i     | 22   | PRO  | N-CA-CB     | -5.08 | 97.91       | 103.25   |
| 51  | 1     | 2777 | G    | N9-C1'-C2'  | 5.08  | 119.62      | 112.00   |
| 17  | Q     | 42   | LYS  | CA-C-N      | 5.08  | 129.59      | 121.62   |
| 17  | Q     | 42   | LYS  | C-N-CA      | 5.08  | 129.59      | 121.62   |
| 51  | 1     | 1087 | G    | N9-C1'-C2'  | 5.05  | 119.57      | 112.00   |
| 48  | x     | 25   | LYS  | N-CA-C      | 5.04  | 121.54      | 110.80   |
| 51  | 1     | 972  | A    | N9-C1'-C2'  | 5.03  | 119.55      | 112.00   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 521   | 0        | 520      | 8       | 0            |
| 2   | B     | 444   | 0        | 461      | 10      | 0            |
| 3   | C     | 409   | 0        | 440      | 3       | 0            |
| 4   | D     | 377   | 0        | 418      | 9       | 0            |
| 5   | E     | 504   | 0        | 574      | 2       | 0            |
| 6   | F     | 302   | 0        | 343      | 5       | 0            |
| 7   | G     | 1704  | 0        | 1732     | 39      | 0            |
| 8   | H     | 1624  | 0        | 1699     | 27      | 0            |
| 9   | I     | 1643  | 0        | 1710     | 34      | 0            |
| 10  | J     | 1156  | 0        | 1199     | 17      | 0            |
| 11  | K     | 817   | 0        | 808      | 16      | 0            |
| 12  | L     | 1181  | 0        | 1240     | 19      | 0            |
| 13  | M     | 979   | 0        | 1034     | 9       | 0            |
| 14  | N     | 1022  | 0        | 1070     | 21      | 0            |
| 15  | O     | 786   | 0        | 828      | 15      | 0            |
| 16  | P     | 869   | 0        | 878      | 20      | 0            |
| 17  | Q     | 955   | 0        | 1019     | 24      | 0            |
| 18  | R     | 883   | 0        | 944      | 20      | 0            |
| 19  | S     | 805   | 0        | 847      | 10      | 0            |
| 20  | T     | 714   | 0        | 737      | 7       | 0            |
| 21  | U     | 649   | 0        | 666      | 16      | 0            |
| 22  | V     | 648   | 0        | 691      | 9       | 0            |
| 23  | W     | 535   | 0        | 552      | 7       | 0            |
| 24  | X     | 637   | 0        | 665      | 8       | 0            |
| 25  | Y     | 665   | 0        | 714      | 12      | 0            |
| 26  | Z     | 544   | 0        | 579      | 12      | 0            |
| 27  | b     | 2082  | 0        | 2157     | 45      | 0            |
| 28  | c     | 1565  | 0        | 1616     | 32      | 0            |
| 29  | d     | 1552  | 0        | 1619     | 27      | 0            |
| 30  | e     | 1410  | 0        | 1447     | 22      | 0            |
| 31  | f     | 1323  | 0        | 1374     | 30      | 0            |
| 32  | g     | 400   | 0        | 423      | 7       | 0            |
| 33  | i     | 1032  | 0        | 1088     | 36      | 0            |
| 34  | j     | 1129  | 0        | 1162     | 20      | 0            |
| 35  | k     | 938   | 0        | 1012     | 19      | 0            |
| 36  | l     | 1045  | 0        | 1117     | 15      | 0            |
| 37  | m     | 1074  | 0        | 1157     | 13      | 0            |
| 38  | n     | 960   | 0        | 1000     | 18      | 0            |
| 39  | o     | 892   | 0        | 923      | 15      | 0            |
| 40  | p     | 917   | 0        | 965      | 12      | 0            |
| 41  | q     | 947   | 0        | 1022     | 10      | 0            |
| 42  | r     | 816   | 0        | 839      | 14      | 0            |
| 43  | s     | 857   | 0        | 922      | 11      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 44  | t     | 738    | 0        | 807      | 9       | 0            |
| 45  | u     | 779    | 0        | 834      | 14      | 0            |
| 46  | v     | 753    | 0        | 780      | 9       | 0            |
| 47  | w     | 575    | 0        | 592      | 9       | 0            |
| 48  | x     | 625    | 0        | 655      | 11      | 0            |
| 49  | y     | 509    | 0        | 543      | 11      | 0            |
| 50  | z     | 449    | 0        | 491      | 9       | 0            |
| 51  | 1     | 62317  | 0        | 31346    | 1455    | 0            |
| 52  | 2     | 2568   | 0        | 1303     | 15      | 0            |
| 53  | 3     | 33012  | 0        | 16618    | 185     | 0            |
| 54  | 4     | 809    | 0        | 404      | 4       | 0            |
| 55  | 8     | 539    | 0        | 305      | 27      | 0            |
| 56  | 9     | 417    | 0        | 224      | 2       | 0            |
| 57  | A1    | 2088   | 0        | 1895     | 24      | 0            |
| 57  | A2    | 2029   | 0        | 1864     | 18      | 0            |
| 58  | B1    | 10353  | 0        | 10548    | 322     | 0            |
| 59  | B2    | 10546  | 0        | 10550    | 164     | 0            |
| 60  | W0    | 650    | 0        | 658      | 10      | 0            |
| 61  | NA    | 2432   | 0        | 1171     | 3       | 0            |
| 62  | NG    | 758    | 0        | 334      | 10      | 0            |
| 63  | 5     | 1622   | 0        | 821      | 28      | 0            |
| 64  | 6     | 1640   | 0        | 837      | 20      | 0            |
| 65  | 0     | 5211   | 0        | 5200     | 46      | 0            |
| 66  | B1    | 1      | 0        | 0        | 0       | 0            |
| 67  | 0     | 37     | 0        | 47       | 0       | 0            |
| 68  | 0     | 28     | 0        | 12       | 0       | 0            |
| All | All   | 181797 | 0        | 131050   | 2821    | 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 9.

All (2821) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:1:275:C:H2'    | 51:1:276:U:H4'    | 1.37                     | 1.07              |
| 51:1:1672:A:C2    | 51:1:2582:G:H5'   | 1.95                     | 1.02              |
| 51:1:1666:G:H2'   | 51:1:1667:G:H5'   | 1.41                     | 1.01              |
| 58:B1:750:PRO:HB3 | 59:B2:549:ASP:OD2 | 1.60                     | 1.01              |
| 51:1:1082:U:H3'   | 51:1:1083:U:H5''  | 1.41                     | 1.00              |
| 51:1:2713:U:H3'   | 51:1:2714:G:H5'   | 1.41                     | 1.00              |
| 51:1:1807:G:H2'   | 51:1:1808:A:H5'   | 1.44                     | 0.99              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:B1:111:THR:HG23 | 58:B1:300:GLN:CD   | 1.86                     | 0.99              |
| 58:B1:352:ARG:HD2  | 59:B2:1268:GLN:NE2 | 1.79                     | 0.98              |
| 51:1:2156:G:H2'    | 51:1:2157:G:H5'    | 1.47                     | 0.95              |
| 58:B1:68:TYR:O     | 58:B1:75:TYR:CE2   | 2.20                     | 0.95              |
| 51:1:1847:A:HO2'   | 51:1:1848:A:H8     | 1.06                     | 0.94              |
| 51:1:644:A:H2'     | 51:1:645:C:H5''    | 1.50                     | 0.93              |
| 51:1:2713:U:H3'    | 51:1:2714:G:C5'    | 1.98                     | 0.93              |
| 51:1:655:A:H4'     | 51:1:656:G:H5'     | 1.50                     | 0.92              |
| 51:1:1102:C:H2'    | 51:1:1103:A:H8     | 1.35                     | 0.92              |
| 51:1:1702:G:H2'    | 51:1:1703:G:H5''   | 1.51                     | 0.92              |
| 54:4:44:G:H21      | 58:B1:427:PRO:HD3  | 1.34                     | 0.91              |
| 30:e:84:ILE:HD13   | 51:1:2312:U:H5'    | 1.51                     | 0.91              |
| 30:e:130:GLY:HA3   | 51:1:2305:U:H5''   | 1.51                     | 0.91              |
| 51:1:1019:U:H3     | 51:1:1142:A:H62    | 1.17                     | 0.91              |
| 51:1:1668:A:H4'    | 51:1:1669:A:H5'    | 1.54                     | 0.90              |
| 51:1:890:C:H2'     | 51:1:891:G:H5'     | 1.53                     | 0.90              |
| 58:B1:68:TYR:C     | 58:B1:75:TYR:HE2   | 1.80                     | 0.89              |
| 58:B1:202:ARG:HG2  | 58:B1:202:ARG:HH11 | 1.34                     | 0.89              |
| 14:N:3:ASN:N       | 14:N:5:TYR:HH      | 1.70                     | 0.89              |
| 63:5:9:A:H2'       | 63:5:11:C:H41      | 1.38                     | 0.89              |
| 51:1:1060:U:H4'    | 51:1:1061:U:H5''   | 1.55                     | 0.88              |
| 51:1:2097:A:H2'    | 51:1:2098:U:C6     | 2.08                     | 0.88              |
| 58:B1:317:THR:HA   | 58:B1:323:PRO:HA   | 1.55                     | 0.88              |
| 59:B2:854:ILE:HG21 | 59:B2:917:SER:HB3  | 1.54                     | 0.88              |
| 65:0:348:THR:HA    | 65:0:359:ARG:HA    | 1.55                     | 0.88              |
| 51:1:11:C:H2'      | 51:1:12:U:H5''     | 1.55                     | 0.87              |
| 51:1:1869:G:H3'    | 51:1:1870:C:H5'    | 1.57                     | 0.86              |
| 2:B:8:THR:HB       | 51:1:2020:A:H5'    | 1.56                     | 0.86              |
| 58:B1:68:TYR:HB3   | 58:B1:75:TYR:OH    | 1.76                     | 0.85              |
| 51:1:2792:A:H2'    | 51:1:2793:C:H5''   | 1.59                     | 0.85              |
| 17:Q:69:GLU:HG3    | 53:3:521:G:H4'     | 1.59                     | 0.85              |
| 51:1:1387:A:H5'    | 51:1:1469:A:H1'    | 1.58                     | 0.84              |
| 51:1:2333:A:H5'    | 51:1:2334:U:H2'    | 1.57                     | 0.84              |
| 51:1:1175:A:H3'    | 51:1:1176:U:H5'    | 1.59                     | 0.83              |
| 51:1:2584:U:H2'    | 51:1:2585:U:H5'    | 1.58                     | 0.83              |
| 58:B1:633:ALA:HB2  | 59:B2:808:ASN:H    | 1.41                     | 0.83              |
| 58:B1:68:TYR:O     | 58:B1:75:TYR:HE2   | 1.58                     | 0.83              |
| 33:i:119:ALA:HB2   | 51:1:1082:U:H5'    | 1.60                     | 0.82              |
| 51:1:475:C:H4'     | 51:1:510:C:H5'     | 1.59                     | 0.82              |
| 51:1:1666:G:C2'    | 51:1:1667:G:H5'    | 2.07                     | 0.82              |
| 55:8:1:DC:H5''     | 58:B1:210:SER:OG   | 1.80                     | 0.82              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1:757:G:H2'     | 51:1:758:C:H5'     | 1.61                     | 0.82              |
| 58:B1:770:LEU:HD13 | 59:B2:618:GLN:HG3  | 1.61                     | 0.82              |
| 51:1:1141:U:H4'    | 51:1:1142:A:O4'    | 1.80                     | 0.82              |
| 51:1:279:A:H61     | 51:1:361:G:H1'     | 1.46                     | 0.81              |
| 51:1:849:A:H2'     | 51:1:850:U:C6      | 2.14                     | 0.81              |
| 51:1:2799:A:H2'    | 51:1:2800:A:H5'    | 1.63                     | 0.81              |
| 51:1:545:U:C2      | 51:1:546:U:H1'     | 2.16                     | 0.81              |
| 51:1:2360:G:H2'    | 51:1:2361:G:H5'    | 1.62                     | 0.81              |
| 58:B1:141:PHE:CE2  | 58:B1:296:LYS:HB2  | 2.16                     | 0.81              |
| 38:n:36:THR:HG22   | 51:1:1278:C:OP1    | 1.80                     | 0.81              |
| 58:B1:37:GLU:O     | 58:B1:61:ILE:HD11  | 1.81                     | 0.81              |
| 51:1:1197:G:O2'    | 51:1:1198:U:H5'    | 1.81                     | 0.80              |
| 51:1:2112:G:H2'    | 51:1:2113:U:H5'    | 1.63                     | 0.80              |
| 51:1:1087:G:N2     | 51:1:1103:A:H1'    | 1.97                     | 0.80              |
| 51:1:2224:G:H4'    | 51:1:2226:C:C2     | 2.16                     | 0.80              |
| 58:B1:144:TYR:HE1  | 58:B1:162:GLU:OE2  | 1.64                     | 0.80              |
| 51:1:1775:U:H2'    | 51:1:1776:G:H5'    | 1.64                     | 0.80              |
| 51:1:784:G:H5'     | 51:1:785:G:OP1     | 1.81                     | 0.80              |
| 58:B1:111:THR:HG23 | 58:B1:300:GLN:OE1  | 1.81                     | 0.80              |
| 58:B1:141:PHE:HE2  | 58:B1:296:LYS:HB2  | 1.45                     | 0.79              |
| 64:6:46:G:H2'      | 64:6:47:U:H5'      | 1.64                     | 0.79              |
| 51:1:1064:C:H41    | 51:1:1069:A:H5''   | 1.47                     | 0.79              |
| 7:G:18:GLN:HG3     | 7:G:189:ASN:HB3    | 1.65                     | 0.79              |
| 51:1:1071:G:O2'    | 51:1:1089:A:H2'    | 1.82                     | 0.79              |
| 3:C:40:PRO:HG3     | 51:1:2348:U:H4'    | 1.63                     | 0.79              |
| 51:1:1297:C:OP1    | 51:1:2710:C:H4'    | 1.82                     | 0.78              |
| 51:1:2286:G:H4'    | 51:1:2287:A:O4'    | 1.83                     | 0.78              |
| 35:k:6:THR:HG22    | 51:1:1666:G:O2'    | 1.83                     | 0.78              |
| 51:1:2130:U:H2'    | 51:1:2131:U:H5''   | 1.65                     | 0.78              |
| 58:B1:186:GLN:HG3  | 58:B1:238:ILE:HG13 | 1.65                     | 0.78              |
| 51:1:275:C:H2'     | 51:1:276:U:C4'     | 2.14                     | 0.78              |
| 51:1:2215:C:H2'    | 51:1:2216:G:C8     | 2.18                     | 0.78              |
| 51:1:2792:A:C3'    | 51:1:2793:C:H5''   | 2.14                     | 0.78              |
| 65:0:508:GLN:HA    | 65:0:513:GLY:CA    | 2.12                     | 0.78              |
| 51:1:1275:A:N6     | 51:1:1296:G:H4'    | 1.99                     | 0.77              |
| 51:1:1310:G:C2'    | 51:1:1311:G:H5'    | 2.14                     | 0.77              |
| 51:1:1536:C:H4'    | 51:1:1537:G:C2     | 2.18                     | 0.77              |
| 65:0:624:PRO:HG2   | 65:0:677:ARG:HD2   | 1.66                     | 0.77              |
| 51:1:1702:G:C2'    | 51:1:1703:G:H5''   | 2.13                     | 0.77              |
| 33:i:55:PRO:HG3    | 51:1:1060:U:OP2    | 1.83                     | 0.77              |
| 55:8:15:DC:H1'     | 58:B1:426:ALA:HB1  | 1.67                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:B1:202:ARG:HG2  | 58:B1:202:ARG:NH1  | 1.99                     | 0.77              |
| 51:1:2156:G:C2'    | 51:1:2157:G:H5'    | 2.14                     | 0.77              |
| 51:1:310:A:O2'     | 51:1:311:A:H2'     | 1.85                     | 0.76              |
| 51:1:1736:U:H2'    | 51:1:1737:G:O4'    | 1.85                     | 0.76              |
| 28:c:114:LYS:HB2   | 51:1:2680:U:OP1    | 1.84                     | 0.76              |
| 55:8:13:DT:H72     | 58:B1:791:ALA:HB2  | 1.66                     | 0.76              |
| 51:1:1394:U:H4'    | 51:1:1603:A:H4'    | 1.66                     | 0.76              |
| 51:1:548:G:H2'     | 51:1:549:G:O4'     | 1.84                     | 0.76              |
| 51:1:368:A:H2'     | 51:1:369:U:H5'     | 1.66                     | 0.76              |
| 51:1:1773:A:H2'    | 51:1:1774:C:H5'    | 1.68                     | 0.76              |
| 51:1:2792:A:C2'    | 51:1:2793:C:H5''   | 2.16                     | 0.75              |
| 51:1:275:C:H3'     | 51:1:276:U:H5''    | 1.66                     | 0.75              |
| 51:1:958:U:H2'     | 52:2:89:U:O2       | 1.87                     | 0.75              |
| 51:1:1063:G:H1     | 51:1:1075:C:N4     | 1.84                     | 0.75              |
| 51:1:1083:U:H2'    | 51:1:1085:A:OP2    | 1.86                     | 0.75              |
| 51:1:1310:G:H2'    | 51:1:1311:G:H5'    | 1.69                     | 0.75              |
| 51:1:2611:C:O2     | 51:1:2611:C:H2'    | 1.86                     | 0.75              |
| 51:1:2432:A:H1'    | 64:6:75:C:O4'      | 1.86                     | 0.75              |
| 58:B1:110:PRO:HG2  | 58:B1:183:GLU:HG3  | 1.69                     | 0.75              |
| 51:1:1020:A:H5'    | 51:1:1021:A:C8     | 2.22                     | 0.74              |
| 51:1:1555:G:H5'    | 51:1:1555:G:H8     | 1.51                     | 0.74              |
| 55:8:3:DC:H2'      | 55:8:4:DT:H72      | 1.69                     | 0.74              |
| 51:1:1061:U:H3'    | 51:1:1062:G:C5'    | 2.18                     | 0.74              |
| 51:1:1425:G:H2'    | 51:1:1426:G:C8     | 2.23                     | 0.74              |
| 51:1:2097:A:H2'    | 51:1:2098:U:H6     | 1.50                     | 0.74              |
| 58:B1:211:GLU:HG2  | 58:B1:215:LYS:HE3  | 1.70                     | 0.73              |
| 51:1:404:A:H1'     | 51:1:406:G:C4      | 2.23                     | 0.73              |
| 58:B1:1143:ASP:OD1 | 58:B1:1148:ARG:NH1 | 2.21                     | 0.73              |
| 51:1:543:G:H2'     | 51:1:544:C:H5''    | 1.68                     | 0.73              |
| 55:8:3:DC:C2'      | 55:8:4:DT:H72      | 2.19                     | 0.73              |
| 31:f:15:ASP:HB3    | 31:f:26:LYS:H      | 1.54                     | 0.73              |
| 51:1:322:A:H5'     | 51:1:340:A:C1'     | 2.19                     | 0.73              |
| 51:1:1433:A:H2'    | 51:1:1434:A:O4'    | 1.89                     | 0.73              |
| 51:1:1670:C:H2'    | 51:1:1671:U:H5'    | 1.70                     | 0.73              |
| 63:5:30:G:H2'      | 63:5:31:A:C8       | 2.24                     | 0.73              |
| 17:Q:33:CYS:HA     | 17:Q:54:VAL:HG12   | 1.70                     | 0.73              |
| 58:B1:105:ILE:HD12 | 58:B1:242:LEU:HD22 | 1.71                     | 0.73              |
| 64:6:50:U:H2'      | 64:6:51:C:C4       | 2.24                     | 0.73              |
| 53:3:456:A:H61     | 53:3:476:U:H3      | 1.36                     | 0.73              |
| 51:1:545:U:H2'     | 51:1:546:U:O4'     | 1.88                     | 0.72              |
| 51:1:481:G:H1'     | 51:1:506:G:N2      | 2.04                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:B1:157:GLN:OE1  | 58:B1:157:GLN:HA   | 1.89                     | 0.72              |
| 65:0:508:GLN:HA    | 65:0:513:GLY:HA2   | 1.69                     | 0.72              |
| 51:1:2713:U:C3'    | 51:1:2714:G:C5'    | 2.67                     | 0.72              |
| 58:B1:210:SER:HB3  | 58:B1:213:LYS:HB2  | 1.71                     | 0.72              |
| 58:B1:220:ARG:HG2  | 58:B1:220:ARG:HH11 | 1.55                     | 0.72              |
| 51:1:633:A:H2'     | 51:1:634:C:H5'     | 1.72                     | 0.72              |
| 51:1:1942:C:H3'    | 51:1:1943:U:H2'    | 1.70                     | 0.72              |
| 51:1:1795:C:H2'    | 51:1:1796:U:O4'    | 1.90                     | 0.72              |
| 51:1:2834:G:H2'    | 51:1:2879:A:H61    | 1.54                     | 0.72              |
| 51:1:394:C:H2'     | 51:1:395:U:O4'     | 1.90                     | 0.72              |
| 51:1:2036:C:H2'    | 51:1:2037:A:C8     | 2.23                     | 0.72              |
| 51:1:2671:G:H2'    | 51:1:2672:U:C6     | 2.25                     | 0.71              |
| 58:B1:107:LEU:HD11 | 58:B1:242:LEU:HB2  | 1.70                     | 0.71              |
| 58:B1:282:LEU:HA   | 58:B1:286:ALA:HA   | 1.70                     | 0.71              |
| 36:l:59:ARG:HD2    | 51:1:250:G:H4'     | 1.71                     | 0.71              |
| 51:1:1858:A:H1'    | 51:1:1885:A:C2     | 2.26                     | 0.71              |
| 58:B1:395:LYS:HZ2  | 58:B1:399:LYS:CD   | 2.03                     | 0.71              |
| 51:1:1441:G:H2'    | 51:1:1442:U:C6     | 2.25                     | 0.71              |
| 53:3:452:A:H61     | 53:3:480:U:H3      | 1.37                     | 0.71              |
| 58:B1:68:TYR:C     | 58:B1:75:TYR:CE2   | 2.65                     | 0.71              |
| 58:B1:93:THR:HB    | 58:B1:97:VAL:HG21  | 1.73                     | 0.71              |
| 51:1:1670:C:C2'    | 51:1:1671:U:H5'    | 2.21                     | 0.71              |
| 51:1:2151:U:H2'    | 51:1:2152:G:H8     | 1.56                     | 0.71              |
| 51:1:368:A:C2'     | 51:1:369:U:H5'     | 2.20                     | 0.71              |
| 51:1:612:G:H2'     | 51:1:614:A:C8      | 2.26                     | 0.71              |
| 51:1:890:C:C2'     | 51:1:891:G:H5'     | 2.21                     | 0.71              |
| 51:1:940:G:H2'     | 51:1:941:A:H5''    | 1.73                     | 0.71              |
| 51:1:1019:U:H3     | 51:1:1142:A:N6     | 1.89                     | 0.71              |
| 53:3:663:A:H61     | 53:3:742:G:H1      | 1.39                     | 0.70              |
| 58:B1:142:GLU:HG3  | 58:B1:142:GLU:O    | 1.89                     | 0.70              |
| 51:1:864:G:O2'     | 51:1:865:C:H5'     | 1.89                     | 0.70              |
| 27:b:47:ARG:NH2    | 51:1:774:G:H5''    | 2.07                     | 0.70              |
| 51:1:723:C:H2'     | 51:1:724:U:C6      | 2.27                     | 0.70              |
| 42:r:79:ARG:NH1    | 51:1:572:A:OP2     | 2.25                     | 0.70              |
| 33:i:22:PRO:HB3    | 51:1:1067:A:H4'    | 1.72                     | 0.70              |
| 51:1:1983:G:O2'    | 51:1:1984:G:H5'    | 1.92                     | 0.70              |
| 51:1:2626:C:O2'    | 51:1:2627:G:H5'    | 1.91                     | 0.70              |
| 51:1:1386:C:H2'    | 51:1:1387:A:H8     | 1.56                     | 0.70              |
| 51:1:1872:A:H2'    | 51:1:1873:G:O4'    | 1.89                     | 0.70              |
| 51:1:2297:A:N1     | 51:1:2321:U:H5     | 1.89                     | 0.70              |
| 57:A2:294:ASN:HA   | 61:NA:464:ILE:H    | 1.57                     | 0.70              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:1:2267:A:H5''   | 51:1:2268:A:H5''    | 1.74                     | 0.70              |
| 57:A1:297:LYS:CB   | 61:NA:79:ALA:HB1    | 2.22                     | 0.70              |
| 51:1:644:A:C2'     | 51:1:645:C:H5''     | 2.22                     | 0.70              |
| 58:B1:352:ARG:HD2  | 59:B2:1268:GLN:HE22 | 1.55                     | 0.70              |
| 65:0:618:LYS:HG3   | 65:0:643:LYS:HZ3    | 1.55                     | 0.70              |
| 51:1:322:A:H5'     | 51:1:340:A:H1'      | 1.73                     | 0.69              |
| 34:j:7:LYS:HG2     | 51:1:538:A:H4'      | 1.73                     | 0.69              |
| 51:1:1337:G:H2'    | 51:1:1338:G:H8      | 1.57                     | 0.69              |
| 51:1:2092:U:H4'    | 51:1:2093:G:H5''    | 1.75                     | 0.69              |
| 59:B2:65:ASN:HB3   | 59:B2:105:TYR:HB2   | 1.74                     | 0.69              |
| 51:1:402:A:H2'     | 51:1:403:U:H5'      | 1.74                     | 0.69              |
| 51:1:1102:C:H2'    | 51:1:1103:A:C8      | 2.22                     | 0.69              |
| 51:1:1555:G:H5'    | 51:1:1555:G:C8      | 2.27                     | 0.69              |
| 51:1:1565:C:HO2'   | 51:1:1566:A:H8      | 1.41                     | 0.69              |
| 58:B1:128:LEU:HD11 | 58:B1:189:LEU:HG    | 1.73                     | 0.69              |
| 51:1:1292:G:H2'    | 51:1:1293:C:C6      | 2.27                     | 0.69              |
| 51:1:1889:A:H2'    | 51:1:1890:A:H8      | 1.58                     | 0.69              |
| 51:1:2151:U:H2'    | 51:1:2152:G:C8      | 2.27                     | 0.69              |
| 51:1:849:A:H2'     | 51:1:850:U:H6       | 1.58                     | 0.69              |
| 51:1:1137:G:O2'    | 51:1:1138:G:H5'     | 1.92                     | 0.69              |
| 51:1:2403:C:O2'    | 51:1:2404:U:H5'     | 1.92                     | 0.69              |
| 58:B1:243:PRO:HG2  | 59:B2:1332:SER:O    | 1.93                     | 0.69              |
| 36:l:30:THR:HG22   | 51:1:810:U:O4       | 1.93                     | 0.69              |
| 51:1:644:A:H2'     | 51:1:645:C:C5'      | 2.21                     | 0.69              |
| 51:1:2758:A:H2'    | 51:1:2759:G:H5'     | 1.75                     | 0.69              |
| 51:1:2869:G:H2'    | 51:1:2870:C:C6      | 2.28                     | 0.69              |
| 51:1:392:U:H2'     | 51:1:393:C:H6       | 1.58                     | 0.69              |
| 51:1:528:A:C8      | 51:1:528:A:H3'      | 2.27                     | 0.69              |
| 63:5:47:U:H4'      | 63:5:48:C:H5'       | 1.75                     | 0.69              |
| 51:1:2114:A:H2     | 51:1:2167:U:H1'     | 1.58                     | 0.68              |
| 51:1:2747:G:O6     | 51:1:2755:C:H5''    | 1.93                     | 0.68              |
| 58:B1:832:LYS:C    | 58:B1:1242:ARG:HH12 | 2.01                     | 0.68              |
| 51:1:319:G:H1      | 51:1:323:C:H5       | 1.41                     | 0.68              |
| 51:1:1078:U:H2'    | 51:1:1088:A:OP1     | 1.94                     | 0.68              |
| 53:3:437:U:H3      | 53:3:495:A:H62      | 1.41                     | 0.68              |
| 58:B1:39:LYS:O     | 58:B1:273:ILE:CG2   | 2.41                     | 0.68              |
| 58:B1:161:THR:HG22 | 58:B1:164:GLN:HB2   | 1.75                     | 0.68              |
| 50:z:38:GLU:OE2    | 51:1:928:A:H5'      | 1.94                     | 0.68              |
| 51:1:1999:C:H5''   | 51:1:2723:C:O2'     | 1.94                     | 0.68              |
| 51:1:419:U:H2'     | 51:1:420:C:C6       | 2.27                     | 0.68              |
| 51:1:905:A:C2'     | 51:1:906:U:H5'      | 2.23                     | 0.68              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:1:2510:C:N4     | 51:1:2511:U:O4      | 2.27                     | 0.68              |
| 58:B1:111:THR:CG2  | 58:B1:300:GLN:CD    | 2.67                     | 0.68              |
| 51:1:282:A:H2'     | 51:1:283:G:H8       | 1.57                     | 0.68              |
| 51:1:419:U:H2'     | 51:1:420:C:H6       | 1.58                     | 0.68              |
| 53:3:1338:G:H22    | 63:5:29:G:H22       | 1.42                     | 0.68              |
| 51:1:1438:U:O2'    | 51:1:1439:A:H5'     | 1.94                     | 0.68              |
| 51:1:1889:A:H2'    | 51:1:1890:A:C8      | 2.29                     | 0.68              |
| 51:1:1702:G:C3'    | 51:1:1703:G:H5''    | 2.24                     | 0.68              |
| 51:1:246:C:H2'     | 51:1:247:G:H5'      | 1.76                     | 0.67              |
| 51:1:1432:G:O2'    | 51:1:1433:A:H5'     | 1.94                     | 0.67              |
| 8:H:117:ASP:HA     | 8:H:120:THR:HG22    | 1.75                     | 0.67              |
| 52:2:65:U:H3'      | 52:2:108:A:H61      | 1.58                     | 0.67              |
| 58:B1:141:PHE:CD2  | 58:B1:293:ARG:O     | 2.47                     | 0.67              |
| 51:1:466:A:H2'     | 51:1:467:G:H5'      | 1.76                     | 0.67              |
| 51:1:1061:U:H3'    | 51:1:1062:G:H5'     | 1.76                     | 0.67              |
| 58:B1:984:LEU:HB3  | 58:B1:993:GLU:HB2   | 1.76                     | 0.67              |
| 51:1:112:U:H2'     | 51:1:113:U:H5'      | 1.76                     | 0.67              |
| 51:1:226:A:H2'     | 51:1:227:A:O4'      | 1.94                     | 0.67              |
| 51:1:703:U:C2'     | 51:1:704:G:H5'      | 2.25                     | 0.67              |
| 51:1:2898:U:H2'    | 51:1:2899:A:C8      | 2.29                     | 0.67              |
| 55:8:3:DC:C6       | 55:8:4:DT:H72       | 2.29                     | 0.67              |
| 51:1:65:U:H2'      | 51:1:66:C:H6        | 1.59                     | 0.67              |
| 51:1:1717:A:H2'    | 51:1:1718:G:H5'     | 1.77                     | 0.67              |
| 51:1:2233:U:H2'    | 51:1:2234:G:C8      | 2.30                     | 0.67              |
| 9:I:73:ASN:HA      | 9:I:76:LYS:HB2      | 1.77                     | 0.67              |
| 48:x:16:ASN:ND2    | 48:x:26:ARG:HB3     | 2.09                     | 0.67              |
| 58:B1:108:ALA:CB   | 58:B1:279:LEU:HD22  | 2.25                     | 0.67              |
| 58:B1:1355:ARG:NH1 | 58:B1:1369:ARG:HH12 | 1.93                     | 0.67              |
| 37:m:14:LYS:NZ     | 51:1:956:G:N7       | 2.35                     | 0.67              |
| 51:1:2516:A:O2'    | 51:1:2517:C:H5'     | 1.95                     | 0.67              |
| 65:0:104:ARG:HH22  | 65:0:407:GLU:HB3    | 1.57                     | 0.67              |
| 58:B1:108:ALA:HB3  | 58:B1:279:LEU:HD22  | 1.77                     | 0.67              |
| 4:D:37:LYS:HD3     | 4:D:39:ARG:HD3      | 1.77                     | 0.67              |
| 51:1:2157:G:H2'    | 51:1:2158:A:H2      | 1.59                     | 0.67              |
| 55:8:23:DC:H2''    | 55:8:24:DC:C5       | 2.30                     | 0.67              |
| 51:1:521:U:H2'     | 51:1:522:A:C8       | 2.30                     | 0.66              |
| 51:1:905:A:H2'     | 51:1:906:U:H5'      | 1.77                     | 0.66              |
| 51:1:1270:C:H5''   | 51:1:1271:G:H5'     | 1.77                     | 0.66              |
| 51:1:1484:U:H2'    | 51:1:1485:U:C6      | 2.30                     | 0.66              |
| 58:B1:117:LEU:HD12 | 58:B1:117:LEU:O     | 1.94                     | 0.66              |
| 65:0:364:VAL:HA    | 65:0:373:GLU:HA     | 1.77                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1:1063:G:H1     | 51:1:1075:C:H41    | 1.42                     | 0.66              |
| 51:1:1176:U:H2'    | 51:1:1177:G:C8     | 2.29                     | 0.66              |
| 55:8:13:DT:OP2     | 58:B1:791:ALA:HB1  | 1.95                     | 0.66              |
| 51:1:707:G:O2'     | 51:1:708:G:H5'     | 1.94                     | 0.66              |
| 51:1:894:U:H2'     | 51:1:895:U:O4'     | 1.93                     | 0.66              |
| 51:1:2278:A:C3'    | 51:1:2279:G:H5''   | 2.25                     | 0.66              |
| 51:1:528:A:H3'     | 51:1:528:A:H8      | 1.59                     | 0.66              |
| 51:1:2278:A:H3'    | 51:1:2279:G:H5''   | 1.78                     | 0.66              |
| 58:B1:1037:PHE:HB3 | 58:B1:1040:MET:HB2 | 1.78                     | 0.66              |
| 51:1:2555:U:H2'    | 51:1:2556:C:H5'    | 1.77                     | 0.66              |
| 51:1:2733:A:O2'    | 51:1:2734:A:H5'    | 1.96                     | 0.66              |
| 45:u:25:LYS:HD3    | 45:u:36:GLU:HB3    | 1.75                     | 0.66              |
| 51:1:673:C:H2'     | 51:1:674:G:H5'     | 1.77                     | 0.66              |
| 17:Q:47:ALA:HB3    | 17:Q:49:ARG:HE     | 1.60                     | 0.66              |
| 51:1:870:U:C2'     | 51:1:871:U:H5'     | 2.26                     | 0.66              |
| 51:1:1082:U:H3'    | 51:1:1083:U:C5'    | 2.22                     | 0.66              |
| 51:1:1733:G:O2'    | 51:1:1734:G:H5'    | 1.95                     | 0.66              |
| 51:1:1020:A:H1'    | 51:1:1021:A:OP2    | 1.95                     | 0.66              |
| 51:1:2233:U:H2'    | 51:1:2234:G:H8     | 1.59                     | 0.66              |
| 51:1:2625:G:H2'    | 51:1:2626:C:C6     | 2.30                     | 0.66              |
| 51:1:2760:C:O2'    | 51:1:2761:A:H5'    | 1.96                     | 0.66              |
| 51:1:1064:C:N4     | 51:1:1069:A:H5''   | 2.10                     | 0.66              |
| 51:1:2595:G:N2     | 51:1:2598:A:OP2    | 2.23                     | 0.66              |
| 28:c:4:LEU:HD23    | 28:c:29:VAL:HG11   | 1.77                     | 0.65              |
| 36:l:39:LYS:NZ     | 51:1:942:G:OP2     | 2.28                     | 0.65              |
| 51:1:703:U:H2'     | 51:1:704:G:H5'     | 1.77                     | 0.65              |
| 51:1:1746:A:H2'    | 51:1:1747:U:C6     | 2.31                     | 0.65              |
| 51:1:2844:G:H2'    | 51:1:2845:U:C6     | 2.31                     | 0.65              |
| 53:3:85:U:H5''     | 53:3:86:G:H5'      | 1.78                     | 0.65              |
| 51:1:635:C:H2'     | 51:1:636:G:C8      | 2.31                     | 0.65              |
| 51:1:1098:A:H2'    | 51:1:1099:G:H5'    | 1.77                     | 0.65              |
| 51:1:2052:A:O2'    | 51:1:2053:G:H5'    | 1.96                     | 0.65              |
| 58:B1:141:PHE:HD2  | 58:B1:293:ARG:O    | 1.80                     | 0.65              |
| 58:B1:193:ASP:HB3  | 58:B1:196:GLN:HB2  | 1.78                     | 0.65              |
| 7:G:67:LEU:HD12    | 7:G:153:MET:HE1    | 1.77                     | 0.65              |
| 38:n:63:ARG:NE     | 51:1:1454:C:H5'    | 2.10                     | 0.65              |
| 51:1:1270:C:H5''   | 51:1:1271:G:C5'    | 2.25                     | 0.65              |
| 51:1:359:G:O2'     | 51:1:360:U:H5'     | 1.97                     | 0.65              |
| 51:1:414:C:H2'     | 51:1:415:A:C8      | 2.31                     | 0.65              |
| 65:0:508:GLN:HA    | 65:0:513:GLY:HA3   | 1.77                     | 0.65              |
| 17:Q:109:ARG:HH21  | 17:Q:112:ALA:HB3   | 1.60                     | 0.65              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 27:b:227:VAL:HG11  | 51:1:784:G:C2       | 2.31                     | 0.65              |
| 51:1:543:G:H2'     | 51:1:544:C:C5'      | 2.26                     | 0.65              |
| 51:1:2221:G:O2'    | 51:1:2222:C:H5'     | 1.95                     | 0.65              |
| 51:1:2834:G:O2'    | 51:1:2835:A:H5'     | 1.97                     | 0.65              |
| 19:S:38:GLU:HA     | 19:S:41:TRP:HB3     | 1.79                     | 0.65              |
| 51:1:2013:A:H5''   | 51:1:2013:A:H8      | 1.59                     | 0.65              |
| 51:1:536:G:H2'     | 51:1:537:G:H5'      | 1.79                     | 0.65              |
| 51:1:1098:A:C2'    | 51:1:1099:G:H5'     | 2.27                     | 0.65              |
| 51:1:1572:A:O2'    | 51:1:1573:G:H5'     | 1.97                     | 0.65              |
| 51:1:1796:U:H2'    | 51:1:1797:G:H8      | 1.61                     | 0.65              |
| 51:1:2193:G:H2'    | 51:1:2194:U:C6      | 2.32                     | 0.65              |
| 58:B1:975:ILE:HG22 | 58:B1:977:SER:H     | 1.62                     | 0.65              |
| 58:B1:978:ARG:HG2  | 58:B1:1197:ASN:HD21 | 1.61                     | 0.65              |
| 51:1:905:A:O2'     | 51:1:906:U:H5'      | 1.97                     | 0.65              |
| 31:f:154:GLU:HG3   | 31:f:156:TYR:H      | 1.61                     | 0.65              |
| 51:1:613:A:H5''    | 51:1:614:A:C8       | 2.32                     | 0.65              |
| 58:B1:68:TYR:HB3   | 58:B1:75:TYR:CE2    | 2.32                     | 0.65              |
| 51:1:1161:C:H2'    | 51:1:1162:G:H8      | 1.61                     | 0.64              |
| 51:1:1853:A:H2'    | 51:1:1854:A:C8      | 2.32                     | 0.64              |
| 51:1:2290:G:H2'    | 51:1:2291:U:C6      | 2.32                     | 0.64              |
| 51:1:2799:A:C2'    | 51:1:2800:A:H5'     | 2.27                     | 0.64              |
| 4:D:24:THR:HG23    | 4:D:27:GLY:H        | 1.61                     | 0.64              |
| 16:P:87:GLY:H      | 16:P:113:THR:HG22   | 1.62                     | 0.64              |
| 28:c:149:ASN:HB3   | 51:1:2572:A:OP2     | 1.97                     | 0.64              |
| 51:1:488:G:N2      | 51:1:491:G:H5''     | 2.11                     | 0.64              |
| 51:1:1788:C:O2'    | 51:1:1789:A:H5'     | 1.96                     | 0.64              |
| 51:1:256:A:O2'     | 51:1:257:C:H5'      | 1.98                     | 0.64              |
| 51:1:306:U:H2'     | 51:1:307:G:O4'      | 1.98                     | 0.64              |
| 51:1:2792:A:H3'    | 51:1:2793:C:H5''    | 1.80                     | 0.64              |
| 26:Z:32:ARG:HG2    | 26:Z:33:ARG:HG3     | 1.80                     | 0.64              |
| 51:1:2404:U:O2'    | 51:1:2405:G:H5'     | 1.97                     | 0.64              |
| 58:B1:395:LYS:HZ2  | 58:B1:399:LYS:HD3   | 1.61                     | 0.64              |
| 58:B1:918:ILE:HG22 | 59:B2:1280:ALA:HB1  | 1.79                     | 0.64              |
| 51:1:414:C:H2'     | 51:1:415:A:H8       | 1.63                     | 0.64              |
| 51:1:2112:G:C2'    | 51:1:2113:U:H5'     | 2.27                     | 0.64              |
| 43:s:6:LYS:HB2     | 51:1:494:G:H4'      | 1.78                     | 0.64              |
| 51:1:815:C:C2      | 51:1:1193:G:N2      | 2.66                     | 0.64              |
| 51:1:2170:A:H2'    | 51:1:2171:A:O4'     | 1.97                     | 0.64              |
| 55:8:3:DC:C2'      | 55:8:4:DT:C7        | 2.75                     | 0.64              |
| 12:L:59:GLU:HA     | 12:L:62:GLU:HB3     | 1.80                     | 0.64              |
| 51:1:1857:G:H22    | 51:1:1884:G:H2'     | 1.62                     | 0.64              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:1:1921:G:O2'    | 51:1:1922:G:H5'   | 1.98                     | 0.64              |
| 51:1:2469:A:H2'    | 51:1:2470:G:O4'   | 1.98                     | 0.64              |
| 59:B2:314:ASN:HD21 | 59:B2:348:SER:HA  | 1.62                     | 0.64              |
| 59:B2:1282:GLY:HA3 | 60:W0:17:PHE:HE1  | 1.63                     | 0.64              |
| 51:1:622:G:O2'     | 51:1:623:C:H5'    | 1.98                     | 0.64              |
| 51:1:1038:G:H2'    | 51:1:1039:A:C8    | 2.32                     | 0.64              |
| 51:1:1181:U:H2'    | 51:1:1182:G:C8    | 2.33                     | 0.64              |
| 51:1:2073:C:O2'    | 51:1:2074:U:H5'   | 1.98                     | 0.64              |
| 51:1:2114:A:N7     | 51:1:2115:G:H1'   | 2.12                     | 0.64              |
| 16:P:19:VAL:HG22   | 16:P:82:GLU:HB2   | 1.79                     | 0.64              |
| 27:b:106:PRO:HD2   | 27:b:109:LEU:HD22 | 1.79                     | 0.64              |
| 51:1:1666:G:H2'    | 51:1:1667:G:C5'   | 2.24                     | 0.64              |
| 58:B1:162:GLU:HA   | 58:B1:162:GLU:OE1 | 1.97                     | 0.64              |
| 58:B1:461:PHE:HD2  | 59:B2:813:GLU:HB2 | 1.62                     | 0.64              |
| 51:1:1164:C:O2'    | 51:1:1165:A:H5'   | 1.99                     | 0.63              |
| 51:1:1766:G:O2'    | 51:1:1767:G:H5'   | 1.98                     | 0.63              |
| 51:1:870:U:H2'     | 51:1:871:U:H5'    | 1.80                     | 0.63              |
| 51:1:940:G:C3'     | 51:1:941:A:H5''   | 2.28                     | 0.63              |
| 51:1:2811:G:O2'    | 51:1:2812:G:H5'   | 1.97                     | 0.63              |
| 65:0:614:GLU:HB3   | 65:0:690:ALA:HB2  | 1.79                     | 0.63              |
| 11:K:38:ARG:HE     | 11:K:97:THR:HA    | 1.62                     | 0.63              |
| 51:1:65:U:H2'      | 51:1:66:C:C6      | 2.33                     | 0.63              |
| 51:1:2314:A:H2'    | 51:1:2315:G:C8    | 2.33                     | 0.63              |
| 51:1:1149:G:H2'    | 51:1:1150:C:C6    | 2.33                     | 0.63              |
| 51:1:201:C:O2'     | 51:1:202:U:H5'    | 1.97                     | 0.63              |
| 51:1:445:C:H2'     | 51:1:446:G:O4'    | 1.98                     | 0.63              |
| 51:1:1280:G:O2'    | 51:1:1281:G:H5'   | 1.99                     | 0.63              |
| 58:B1:245:LEU:HG   | 58:B1:246:PRO:HD2 | 1.80                     | 0.63              |
| 7:G:173:LYS:O      | 7:G:177:ASN:ND2   | 2.32                     | 0.63              |
| 26:Z:65:ARG:NH2    | 53:3:1087:G:N3    | 2.47                     | 0.63              |
| 34:j:45:THR:HB     | 34:j:48:VAL:HG22  | 1.81                     | 0.63              |
| 51:1:2636:C:H2'    | 51:1:2637:U:H6    | 1.64                     | 0.63              |
| 51:1:2898:U:H2'    | 51:1:2899:A:H8    | 1.64                     | 0.63              |
| 9:I:152:SER:H      | 9:I:155:LYS:HD3   | 1.63                     | 0.63              |
| 51:1:212:G:O2'     | 51:1:213:A:H5'    | 1.99                     | 0.63              |
| 51:1:1909:C:H2'    | 51:1:1910:G:H8    | 1.64                     | 0.63              |
| 51:1:554:U:H2'     | 51:1:555:G:O4'    | 1.99                     | 0.62              |
| 53:3:373:A:H61     | 53:3:391:G:H1'    | 1.64                     | 0.62              |
| 58:B1:128:LEU:HA   | 58:B1:192:MET:HE1 | 1.81                     | 0.62              |
| 1:A:1:MET:HG2      | 52:2:43:C:H5''    | 1.82                     | 0.62              |
| 51:1:317:G:H2'     | 51:1:318:C:H6     | 1.64                     | 0.62              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 45:u:87:GLU:HG2     | 45:u:92:VAL:HG21    | 1.82                     | 0.62              |
| 51:1:1448:G:H2'     | 51:1:1449:G:H8      | 1.64                     | 0.62              |
| 51:1:161:A:N7       | 51:1:162:U:H5       | 1.96                     | 0.62              |
| 51:1:1524:G:H2'     | 51:1:1525:A:H8      | 1.63                     | 0.62              |
| 51:1:2298:A:H2'     | 51:1:2299:U:O4'     | 1.99                     | 0.62              |
| 55:8:13:DT:C7       | 58:B1:791:ALA:HB2   | 2.29                     | 0.62              |
| 51:1:37:C:O2'       | 51:1:38:A:H5'       | 1.99                     | 0.62              |
| 51:1:1680:U:H2'     | 51:1:1681:G:O4'     | 2.00                     | 0.62              |
| 58:B1:285:LEU:HD13  | 58:B1:285:LEU:H     | 1.62                     | 0.62              |
| 58:B1:1355:ARG:NH1  | 58:B1:1369:ARG:NH1  | 2.47                     | 0.62              |
| 64:6:46:G:C2'       | 64:6:47:U:H5'       | 2.29                     | 0.62              |
| 22:V:30:HIS:HD2     | 22:V:33:TYR:H       | 1.48                     | 0.62              |
| 44:t:53:VAL:HG12    | 44:t:92:ASN:HD22    | 1.65                     | 0.62              |
| 51:1:2092:U:H5      | 51:1:2199:A:H2      | 1.48                     | 0.62              |
| 58:B1:100:GLU:HA    | 59:B2:1328:LYS:HE2  | 1.82                     | 0.62              |
| 51:1:872:U:O2'      | 51:1:873:C:H5'      | 1.99                     | 0.62              |
| 51:1:889:C:H2'      | 51:1:890:C:O4'      | 1.99                     | 0.62              |
| 51:1:941:A:H2'      | 51:1:942:G:O4'      | 2.00                     | 0.62              |
| 16:P:45:THR:HG23    | 16:P:48:GLY:H       | 1.65                     | 0.62              |
| 51:1:1935:G:H1'     | 51:1:1964:G:N2      | 2.15                     | 0.62              |
| 58:B1:111:THR:CG2   | 58:B1:300:GLN:NE2   | 2.63                     | 0.62              |
| 51:1:161:A:H3'      | 51:1:162:U:H5''     | 1.81                     | 0.61              |
| 51:1:2345:G:N3      | 51:1:2381:A:H2'     | 2.15                     | 0.61              |
| 51:1:2734:A:H2'     | 51:1:2735:G:H5'     | 1.82                     | 0.61              |
| 55:8:3:DC:H2'       | 55:8:4:DT:C7        | 2.30                     | 0.61              |
| 59:B2:55:SER:OG     | 59:B2:465:ARG:NH1   | 2.33                     | 0.61              |
| 4:D:3:ARG:O         | 4:D:6:GLN:NE2       | 2.34                     | 0.61              |
| 16:P:58:THR:HG22    | 16:P:60:PHE:H       | 1.65                     | 0.61              |
| 32:g:50:ARG:HH22    | 32:g:51:ARG:HH21    | 1.48                     | 0.61              |
| 37:m:86:LYS:NZ      | 51:1:955:U:OP1      | 2.32                     | 0.61              |
| 7:G:15:PHE:HB2      | 7:G:39:ILE:HG23     | 1.82                     | 0.61              |
| 51:1:172:A:H2'      | 51:1:173:A:H8       | 1.66                     | 0.61              |
| 55:8:1:DC:H2''      | 55:8:2:DC:C5        | 2.35                     | 0.61              |
| 58:B1:633:ALA:HA    | 59:B2:806:PRO:O     | 2.01                     | 0.61              |
| 58:B1:1357:ILE:HD11 | 59:B2:1287:LEU:HD13 | 1.80                     | 0.61              |
| 2:B:43:THR:HG1      | 2:B:46:GLY:H        | 1.48                     | 0.61              |
| 51:1:322:A:H5'      | 51:1:340:A:O4'      | 2.00                     | 0.61              |
| 51:1:940:G:C2'      | 51:1:941:A:H5''     | 2.30                     | 0.61              |
| 51:1:2404:U:H2'     | 51:1:2405:G:O4'     | 2.01                     | 0.61              |
| 51:1:590:A:O2'      | 51:1:591:U:H5'      | 2.00                     | 0.61              |
| 51:1:1040:A:H2      | 51:1:1115:G:H22     | 1.48                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1:1086:A:H5'    | 51:1:1103:A:H2     | 1.65                     | 0.61              |
| 51:1:1503:A:H3'    | 51:1:1504:A:H5''   | 1.81                     | 0.61              |
| 57:A1:211:ILE:HG12 | 57:A1:219:ARG:HH12 | 1.65                     | 0.61              |
| 58:B1:68:TYR:HB3   | 58:B1:75:TYR:CZ    | 2.35                     | 0.61              |
| 51:1:236:C:H2'     | 51:1:237:C:H6      | 1.64                     | 0.61              |
| 51:1:547:A:H3'     | 51:1:547:A:N3      | 2.16                     | 0.61              |
| 51:1:558:U:H6      | 51:1:558:U:O5'     | 1.84                     | 0.61              |
| 51:1:723:C:H2'     | 51:1:724:U:H6      | 1.64                     | 0.61              |
| 51:1:1717:A:C2'    | 51:1:1718:G:H5'    | 2.30                     | 0.61              |
| 51:1:2188:U:H2'    | 51:1:2189:U:O4'    | 2.01                     | 0.61              |
| 58:B1:395:LYS:NZ   | 58:B1:399:LYS:HD3  | 2.15                     | 0.61              |
| 51:1:435:C:H2'     | 51:1:436:C:H5'     | 1.82                     | 0.61              |
| 51:1:2097:A:H2'    | 51:1:2098:U:O4'    | 2.00                     | 0.61              |
| 28:c:181:ASP:HB3   | 28:c:186:LEU:HB2   | 1.82                     | 0.61              |
| 51:1:1775:U:C2'    | 51:1:1776:G:H5'    | 2.30                     | 0.61              |
| 51:1:2804:U:H2'    | 51:1:2805:C:C6     | 2.36                     | 0.61              |
| 58:B1:201:LEU:HB2  | 58:B1:221:ILE:HD13 | 1.80                     | 0.61              |
| 18:R:102:LYS:HG2   | 18:R:103:THR:HG23  | 1.83                     | 0.60              |
| 34:j:132:HIS:CD2   | 51:1:7:G:H5'       | 2.35                     | 0.60              |
| 51:1:198:C:H42     | 51:1:248:G:H1      | 1.49                     | 0.60              |
| 51:1:2637:U:H2'    | 51:1:2638:G:H5'    | 1.82                     | 0.60              |
| 51:1:2852:G:O2'    | 51:1:2853:C:H5'    | 2.01                     | 0.60              |
| 51:1:854:C:O2'     | 51:1:855:G:H5'     | 2.01                     | 0.60              |
| 51:1:1954:G:H1'    | 51:1:1956:U:O4     | 2.01                     | 0.60              |
| 51:1:2327:A:H2'    | 51:1:2328:A:C8     | 2.35                     | 0.60              |
| 34:j:39:LYS:HE3    | 51:1:1009:A:OP1    | 2.01                     | 0.60              |
| 37:m:17:ASN:O      | 37:m:38:ARG:NH1    | 2.34                     | 0.60              |
| 51:1:1198:U:H2'    | 51:1:1199:U:C6     | 2.37                     | 0.60              |
| 51:1:2812:G:H2'    | 51:1:2813:A:C8     | 2.36                     | 0.60              |
| 58:B1:154:LEU:HD21 | 58:B1:160:LEU:HD21 | 1.83                     | 0.60              |
| 58:B1:223:LEU:HG   | 58:B1:223:LEU:O    | 2.00                     | 0.60              |
| 58:B1:770:LEU:HD13 | 59:B2:618:GLN:CG   | 2.30                     | 0.60              |
| 57:A1:38:THR:HB    | 57:A2:45:ARG:HD3   | 1.82                     | 0.60              |
| 58:B1:951:GLN:NE2  | 58:B1:1014:GLY:O   | 2.35                     | 0.60              |
| 51:1:1437:C:H2'    | 51:1:1438:U:C6     | 2.36                     | 0.60              |
| 53:3:1032:G:H21    | 53:3:1033:G:H4'    | 1.65                     | 0.60              |
| 29:d:149:ILE:HG23  | 29:d:188:MET:HB3   | 1.83                     | 0.60              |
| 33:i:135:MET:HE2   | 51:1:1062:G:H21    | 1.65                     | 0.60              |
| 51:1:2093:G:O2'    | 51:1:2094:A:H5'    | 2.01                     | 0.60              |
| 53:3:1133:G:H1     | 53:3:1141:C:H42    | 1.48                     | 0.60              |
| 58:B1:1161:GLY:HA3 | 58:B1:1179:PRO:HA  | 1.82                     | 0.60              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:1:1026:G:H2'    | 51:1:1027:A:H8      | 1.67                     | 0.60              |
| 51:1:1508:A:H2'    | 51:1:1509:A:O4'     | 2.01                     | 0.60              |
| 51:1:1553:A:HO2'   | 51:1:1554:U:H5      | 1.48                     | 0.60              |
| 51:1:1775:U:H2'    | 51:1:1776:G:C5'     | 2.29                     | 0.60              |
| 55:8:7:DC:H2''     | 55:8:8:DT:H71       | 1.84                     | 0.60              |
| 22:V:11:VAL:HA     | 22:V:22:VAL:HA      | 1.83                     | 0.60              |
| 47:w:38:GLY:HA2    | 51:1:2330:G:H21     | 1.66                     | 0.60              |
| 51:1:2137:U:H2'    | 51:1:2138:G:H8      | 1.67                     | 0.60              |
| 53:3:1040:U:H2'    | 53:3:1041:G:H8      | 1.67                     | 0.60              |
| 57:A1:112:ALA:HB3  | 57:A1:126:PRO:HA    | 1.83                     | 0.60              |
| 58:B1:370:LYS:HG2  | 58:B1:441:LEU:HD23  | 1.84                     | 0.60              |
| 58:B1:926:PRO:HG2  | 58:B1:1248:ILE:HD11 | 1.84                     | 0.60              |
| 51:1:794:A:H2'     | 51:1:795:C:O4'      | 2.02                     | 0.60              |
| 51:1:893:C:H2'     | 51:1:894:U:C6       | 2.36                     | 0.60              |
| 51:1:1183:U:H2'    | 51:1:1184:U:C6      | 2.37                     | 0.60              |
| 51:1:1287:A:C5     | 51:1:1288:G:C6      | 2.89                     | 0.60              |
| 51:1:2187:U:O2'    | 51:1:2188:U:H5'     | 2.02                     | 0.60              |
| 53:3:148:G:H1'     | 53:3:1447:A:H1'     | 1.84                     | 0.60              |
| 53:3:1351:U:H3     | 53:3:1371:G:H1      | 1.49                     | 0.60              |
| 55:8:11:DC:H2'     | 55:8:12:DG:C8       | 2.37                     | 0.60              |
| 58:B1:342:LEU:HD23 | 58:B1:1352:ILE:HG23 | 1.83                     | 0.60              |
| 59:B2:120:GLN:NE2  | 59:B2:490:GLN:OE1   | 2.32                     | 0.60              |
| 51:1:2360:G:C2'    | 51:1:2361:G:H5'     | 2.31                     | 0.60              |
| 58:B1:412:LEU:HD22 | 58:B1:441:LEU:HD21  | 1.84                     | 0.60              |
| 59:B2:528:ARG:NH2  | 59:B2:576:SER:O     | 2.30                     | 0.60              |
| 59:B2:1072:ASN:ND2 | 59:B2:1111:GLN:OE1  | 2.35                     | 0.60              |
| 51:1:1670:C:H2'    | 51:1:1671:U:C5'     | 2.31                     | 0.59              |
| 51:1:1773:A:C2'    | 51:1:1774:C:H5'     | 2.31                     | 0.59              |
| 58:B1:99:ARG:NH1   | 58:B1:99:ARG:HG3    | 2.17                     | 0.59              |
| 51:1:283:G:H2'     | 51:1:284:U:H5'      | 1.83                     | 0.59              |
| 14:N:79:ARG:HH21   | 14:N:102:PHE:HA     | 1.67                     | 0.59              |
| 33:i:19:PRO:HA     | 33:i:24:GLY:HA3     | 1.85                     | 0.59              |
| 51:1:1071:G:H1'    | 51:1:1089:A:C8      | 2.37                     | 0.59              |
| 51:1:1538:G:H2'    | 51:1:1539:U:C6      | 2.37                     | 0.59              |
| 51:1:1857:G:N2     | 51:1:1884:G:H2'     | 2.17                     | 0.59              |
| 51:1:2661:G:H5'    | 65:0:19:ILE:HD13    | 1.85                     | 0.59              |
| 55:8:9:DG:H4'      | 58:B1:120:LEU:HG    | 1.84                     | 0.59              |
| 51:1:11:C:C2'      | 51:1:12:U:H5''      | 2.29                     | 0.59              |
| 51:1:851:C:H2'     | 51:1:852:U:C6       | 2.36                     | 0.59              |
| 51:1:2386:A:O2'    | 51:1:2387:U:H5'     | 2.01                     | 0.59              |
| 24:X:30:LEU:HB2    | 24:X:48:ILE:HG22    | 1.84                     | 0.59              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 27:b:153:LEU:HD23  | 51:1:1799:G:C2      | 2.37                     | 0.59              |
| 51:1:2643:G:H2'    | 51:1:2644:G:H5'     | 1.84                     | 0.59              |
| 51:1:2743:U:H3'    | 51:1:2744:G:H5''    | 1.84                     | 0.59              |
| 51:1:2789:C:H2'    | 51:1:2893:A:N7      | 2.18                     | 0.59              |
| 59:B2:918:LEU:O    | 59:B2:918:LEU:HD23  | 2.02                     | 0.59              |
| 30:e:51:ASN:OD1    | 30:e:149:ARG:NH1    | 2.34                     | 0.59              |
| 39:o:4:LYS:HD3     | 39:o:7:ARG:HH21     | 1.65                     | 0.59              |
| 51:1:841:G:O2'     | 51:1:842:U:H5'      | 2.02                     | 0.59              |
| 51:1:1130:U:O2'    | 51:1:1131:G:OP1     | 2.20                     | 0.59              |
| 51:1:2717:C:C4     | 51:1:2718:G:N7      | 2.70                     | 0.59              |
| 29:d:77:ILE:HG23   | 51:1:1256:G:H21     | 1.68                     | 0.59              |
| 51:1:2165:C:H2'    | 51:1:2166:U:C6      | 2.38                     | 0.59              |
| 29:d:68:ALA:HA     | 51:1:1255:U:C5      | 2.37                     | 0.59              |
| 45:u:40:LEU:HD12   | 45:u:59:GLU:HG2     | 1.84                     | 0.59              |
| 51:1:2153:C:H2'    | 51:1:2154:A:H5'     | 1.85                     | 0.59              |
| 51:1:2749:A:OP2    | 51:1:2751:G:H5''    | 2.02                     | 0.59              |
| 58:B1:201:LEU:HD11 | 58:B1:220:ARG:HH11  | 1.67                     | 0.59              |
| 58:B1:725:MET:SD   | 59:B2:1101:LEU:HD23 | 2.42                     | 0.59              |
| 58:B1:750:PRO:CB   | 59:B2:549:ASP:OD2   | 2.45                     | 0.59              |
| 65:0:557:ILE:HG21  | 65:0:576:ILE:HD12   | 1.85                     | 0.59              |
| 9:I:69:ARG:NH1     | 53:3:401:C:OP2      | 2.36                     | 0.59              |
| 9:I:201:GLU:O      | 53:3:8:A:N6         | 2.36                     | 0.59              |
| 30:e:9:ASP:N       | 30:e:9:ASP:OD1      | 2.33                     | 0.59              |
| 51:1:1042:G:H2'    | 51:1:1043:C:C6      | 2.37                     | 0.59              |
| 59:B2:1142:ARG:NH1 | 59:B2:1161:LEU:O    | 2.36                     | 0.59              |
| 14:N:17:ARG:HB2    | 14:N:65:THR:HG23    | 1.83                     | 0.59              |
| 27:b:34:GLU:HG3    | 27:b:63:ILE:HD11    | 1.84                     | 0.59              |
| 34:j:116:ARG:NH2   | 51:1:529:A:OP2      | 2.32                     | 0.59              |
| 51:1:528:A:C8      | 51:1:528:A:C3'      | 2.86                     | 0.59              |
| 51:1:1171:G:H2'    | 51:1:1172:C:O4'     | 2.02                     | 0.59              |
| 58:B1:161:THR:HG23 | 58:B1:164:GLN:H     | 1.68                     | 0.59              |
| 58:B1:438:GLU:HG3  | 58:B1:485:MET:HE1   | 1.85                     | 0.59              |
| 28:c:55:LYS:NZ     | 28:c:59:ARG:O       | 2.36                     | 0.58              |
| 29:d:77:ILE:CG2    | 51:1:1256:G:H21     | 2.15                     | 0.58              |
| 34:j:3:THR:N       | 51:1:995:C:N3       | 2.48                     | 0.58              |
| 51:1:246:C:C2'     | 51:1:247:G:H5'      | 2.33                     | 0.58              |
| 51:1:1077:A:C8     | 51:1:1078:U:H1'     | 2.38                     | 0.58              |
| 51:1:1337:G:H2'    | 51:1:1338:G:C8      | 2.38                     | 0.58              |
| 51:1:1524:G:H2'    | 51:1:1525:A:C8      | 2.38                     | 0.58              |
| 51:1:2533:U:H2'    | 51:1:2534:A:H5'     | 1.85                     | 0.58              |
| 47:w:40:LYS:HE3    | 51:1:2330:G:O2'     | 2.03                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1:1333:G:O2'    | 51:1:1334:G:H5'    | 2.03                     | 0.58              |
| 51:1:1725:U:H2'    | 51:1:1726:C:C6     | 2.38                     | 0.58              |
| 51:1:2183:A:H2'    | 51:1:2184:A:C4     | 2.37                     | 0.58              |
| 51:1:49:A:H5''     | 51:1:51:G:O4'      | 2.02                     | 0.58              |
| 51:1:1469:A:H2'    | 51:1:1470:A:C8     | 2.38                     | 0.58              |
| 51:1:2834:G:H2'    | 51:1:2879:A:N6     | 2.17                     | 0.58              |
| 53:3:422:C:O2'     | 53:3:423:G:N2      | 2.36                     | 0.58              |
| 15:O:46:LYS:HG2    | 15:O:68:ARG:HG2    | 1.84                     | 0.58              |
| 42:r:4:VAL:HG22    | 42:r:40:MET:HG2    | 1.84                     | 0.58              |
| 51:1:834:G:H2'     | 51:1:835:C:O4'     | 2.04                     | 0.58              |
| 51:1:1098:A:H2'    | 51:1:1099:G:C5'    | 2.33                     | 0.58              |
| 51:1:2215:C:H2'    | 51:1:2216:G:H8     | 1.65                     | 0.58              |
| 59:B2:707:ALA:O    | 59:B2:711:ASP:HB2  | 2.04                     | 0.58              |
| 65:O:618:LYS:HG3   | 65:O:643:LYS:NZ    | 2.19                     | 0.58              |
| 21:U:70:ARG:HH22   | 53:3:451:A:H5'     | 1.66                     | 0.58              |
| 51:1:1511:G:H2'    | 51:1:1512:C:C6     | 2.38                     | 0.58              |
| 51:1:1561:C:H2'    | 51:1:1562:U:C6     | 2.39                     | 0.58              |
| 51:1:2812:G:H2'    | 51:1:2813:A:H8     | 1.68                     | 0.58              |
| 58:B1:514:THR:HG21 | 58:B1:596:LEU:HD12 | 1.84                     | 0.58              |
| 51:1:146:A:H2'     | 51:1:147:C:C6      | 2.39                     | 0.58              |
| 51:1:215:G:H4'     | 51:1:216:A:H4'     | 1.84                     | 0.58              |
| 51:1:1400:U:O2'    | 51:1:1401:G:H5'    | 2.04                     | 0.58              |
| 58:B1:275:ARG:NH1  | 58:B1:278:ARG:NH1  | 2.51                     | 0.58              |
| 51:1:1845:G:O2'    | 51:1:1846:G:H5'    | 2.02                     | 0.58              |
| 58:B1:144:TYR:CE1  | 58:B1:162:GLU:OE2  | 2.51                     | 0.58              |
| 23:W:49:LYS:HA     | 23:W:52:ARG:HH21   | 1.69                     | 0.58              |
| 30:e:47:LYS:O      | 30:e:51:ASN:ND2    | 2.37                     | 0.58              |
| 51:1:640:C:O2'     | 51:1:641:U:H5'     | 2.04                     | 0.58              |
| 51:1:1579:A:H2'    | 51:1:1580:A:C8     | 2.38                     | 0.58              |
| 51:1:1893:C:H2'    | 51:1:1894:C:H5'    | 1.86                     | 0.58              |
| 51:1:2636:C:H2'    | 51:1:2637:U:C6     | 2.39                     | 0.58              |
| 53:3:409:U:H3      | 53:3:433:G:H1      | 1.51                     | 0.58              |
| 58:B1:97:VAL:HG11  | 58:B1:101:ARG:NH2  | 2.18                     | 0.58              |
| 58:B1:198:CYS:HA   | 58:B1:221:ILE:HD11 | 1.86                     | 0.58              |
| 58:B1:1361:THR:HB  | 59:B2:1284:ALA:HB3 | 1.86                     | 0.58              |
| 9:I:10:LEU:HD23    | 9:I:62:ARG:HB3     | 1.86                     | 0.58              |
| 19:S:5:MET:HE1     | 53:3:981:U:H5''    | 1.86                     | 0.58              |
| 29:d:1:MET:HG2     | 29:d:16:GLU:HG2    | 1.86                     | 0.58              |
| 51:1:673:C:C2'     | 51:1:674:G:H5'     | 2.34                     | 0.58              |
| 51:1:1565:C:O2'    | 51:1:1566:A:H8     | 1.87                     | 0.58              |
| 51:1:2762:C:H2'    | 51:1:2763:G:H5'    | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:45:THR:O      | 7:G:49:PHE:N      | 2.35                     | 0.57              |
| 27:b:141:HIS:ND1  | 27:b:192:GLY:O    | 2.35                     | 0.57              |
| 39:o:56:LYS:NZ    | 52:2:117:G:OP1    | 2.36                     | 0.57              |
| 51:1:1275:A:C6    | 51:1:1296:G:H4'   | 2.39                     | 0.57              |
| 51:1:1526:C:H2'   | 51:1:1527:G:O4'   | 2.04                     | 0.57              |
| 51:1:2899:A:O2'   | 51:1:2900:A:H5'   | 2.04                     | 0.57              |
| 58:B1:99:ARG:CG   | 58:B1:99:ARG:HH11 | 2.17                     | 0.57              |
| 65:0:94:ASP:HB3   | 65:0:465:HIS:HB2  | 1.85                     | 0.57              |
| 27:b:157:ALA:O    | 51:1:1820:U:C2    | 2.56                     | 0.57              |
| 27:b:220:ARG:NH1  | 51:1:1789:A:OP2   | 2.38                     | 0.57              |
| 28:c:63:PRO:HG3   | 51:1:2787:C:H1'   | 1.85                     | 0.57              |
| 37:m:66:ARG:NH1   | 37:m:104:GLU:OE2  | 2.36                     | 0.57              |
| 38:n:63:ARG:CZ    | 51:1:1454:C:H5'   | 2.34                     | 0.57              |
| 49:y:39:GLN:HG2   | 51:1:96:C:OP1     | 2.05                     | 0.57              |
| 51:1:32:C:H2'     | 51:1:33:C:C6      | 2.39                     | 0.57              |
| 51:1:163:C:H2'    | 51:1:164:C:O4'    | 2.05                     | 0.57              |
| 51:1:1463:C:H2'   | 51:1:1464:G:H8    | 1.68                     | 0.57              |
| 58:B1:42:GLU:HB3  | 58:B1:52:GLU:HG3  | 1.86                     | 0.57              |
| 45:u:36:GLU:HA    | 45:u:61:GLU:HG2   | 1.86                     | 0.57              |
| 51:1:1108:U:H2'   | 51:1:1109:C:C2    | 2.40                     | 0.57              |
| 58:B1:615:LYS:HG2 | 60:W0:5:THR:HG21  | 1.85                     | 0.57              |
| 1:A:26:SER:OG     | 1:A:27:THR:N      | 2.37                     | 0.57              |
| 16:P:111:ASP:HB2  | 26:Z:16:ARG:HH22  | 1.68                     | 0.57              |
| 25:Y:59:ARG:NH1   | 53:3:177:G:OP1    | 2.37                     | 0.57              |
| 38:n:22:ARG:HG3   | 38:n:70:THR:HA    | 1.86                     | 0.57              |
| 57:A2:28:LEU:HB2  | 57:A2:201:LEU:HB3 | 1.85                     | 0.57              |
| 59:B2:69:GLN:HE21 | 59:B2:101:ARG:HD2 | 1.67                     | 0.57              |
| 51:1:621:A:H2'    | 51:1:622:G:H5'    | 1.86                     | 0.57              |
| 51:1:1173:U:C5    | 51:1:1174:U:H1'   | 2.40                     | 0.57              |
| 51:1:1528:A:H2'   | 51:1:1529:G:H5'   | 1.87                     | 0.57              |
| 39:o:25:ARG:NH1   | 52:2:8:C:O3'      | 2.37                     | 0.57              |
| 51:1:593:U:H2'    | 51:1:594:U:C6     | 2.40                     | 0.57              |
| 51:1:1319:C:O2'   | 51:1:1320:C:H5'   | 2.05                     | 0.57              |
| 51:1:2186:G:O2'   | 51:1:2187:U:H5'   | 2.04                     | 0.57              |
| 58:B1:37:GLU:O    | 58:B1:61:ILE:CD1  | 2.52                     | 0.57              |
| 58:B1:638:SER:OG  | 58:B1:639:VAL:N   | 2.36                     | 0.57              |
| 25:Y:73:ARG:NH2   | 53:3:261:U:OP2    | 2.36                     | 0.57              |
| 28:c:129:THR:OG1  | 28:c:140:HIS:O    | 2.22                     | 0.57              |
| 51:1:74:A:H4'     | 51:1:75:G:O5'     | 2.05                     | 0.57              |
| 51:1:235:U:H2'    | 51:1:236:C:C6     | 2.39                     | 0.57              |
| 51:1:635:C:H2'    | 51:1:636:G:H8     | 1.70                     | 0.57              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:1:1520:U:O2'    | 51:1:1521:G:H5'     | 2.05                     | 0.57              |
| 51:1:2897:U:H2'    | 51:1:2898:U:C6      | 2.39                     | 0.57              |
| 58:B1:241:VAL:O    | 58:B1:241:VAL:HG12  | 2.04                     | 0.57              |
| 58:B1:510:LEU:HD22 | 58:B1:601:ILE:HD12  | 1.86                     | 0.57              |
| 21:U:55:ASP:OD1    | 21:U:55:ASP:N       | 2.38                     | 0.57              |
| 38:n:54:LEU:HD23   | 38:n:66:ALA:HB2     | 1.86                     | 0.57              |
| 41:q:30:VAL:HG13   | 51:1:580:U:O3'      | 2.04                     | 0.57              |
| 51:1:287:G:H2'     | 51:1:288:U:C6       | 2.40                     | 0.57              |
| 51:1:366:C:O2'     | 51:1:367:G:H5'      | 2.04                     | 0.57              |
| 51:1:2092:U:H4'    | 51:1:2093:G:C5'     | 2.34                     | 0.57              |
| 8:H:76:ILE:HD11    | 54:4:23:U:H4'       | 1.87                     | 0.57              |
| 27:b:259:ASN:ND2   | 27:b:262:THR:OG1    | 2.38                     | 0.57              |
| 51:1:323:C:H3'     | 51:1:323:C:OP2      | 2.05                     | 0.57              |
| 51:1:327:G:O2'     | 51:1:328:U:H5'      | 2.04                     | 0.57              |
| 53:3:1125:U:H2'    | 53:3:1126:U:H2'     | 1.85                     | 0.57              |
| 57:A2:82:LEU:HD11  | 57:A2:171:LEU:HD23  | 1.86                     | 0.57              |
| 58:B1:741:ALA:O    | 58:B1:762:ASN:ND2   | 2.38                     | 0.57              |
| 59:B2:1122:LYS:NZ  | 59:B2:1126:ASP:OD1  | 2.38                     | 0.57              |
| 51:1:69:C:H2'      | 51:1:70:G:H8        | 1.70                     | 0.56              |
| 51:1:503:A:H4'     | 51:1:505:A:H5'      | 1.87                     | 0.56              |
| 59:B2:1142:ARG:NH2 | 59:B2:1166:ASP:OD1  | 2.38                     | 0.56              |
| 40:p:1:SER:OG      | 40:p:2:ASN:N        | 2.37                     | 0.56              |
| 51:1:2570:G:H2'    | 51:1:2571:U:H5'     | 1.85                     | 0.56              |
| 51:1:2662:A:H2'    | 51:1:2663:G:O4'     | 2.05                     | 0.56              |
| 59:B2:818:VAL:HG22 | 59:B2:1096:ILE:HG12 | 1.87                     | 0.56              |
| 7:G:114:LYS:HE3    | 7:G:151:LYS:HB2     | 1.86                     | 0.56              |
| 10:J:54:GLU:HG2    | 10:J:56:PRO:HD2     | 1.86                     | 0.56              |
| 18:R:100:ARG:NH1   | 18:R:103:THR:OG1    | 2.38                     | 0.56              |
| 35:k:65:THR:HG23   | 35:k:68:GLY:H       | 1.69                     | 0.56              |
| 46:v:57:TYR:OH     | 46:v:79:ARG:NH2     | 2.38                     | 0.56              |
| 50:z:4:ILE:HD11    | 50:z:58:GLU:HG2     | 1.86                     | 0.56              |
| 51:1:184:C:H2'     | 51:1:185:G:H8       | 1.70                     | 0.56              |
| 51:1:358:U:H2'     | 51:1:359:G:C8       | 2.41                     | 0.56              |
| 51:1:543:G:H2'     | 51:1:544:C:O4'      | 2.05                     | 0.56              |
| 51:1:727:A:H2'     | 51:1:728:G:C8       | 2.40                     | 0.56              |
| 51:1:2845:U:H2'    | 51:1:2846:G:H8      | 1.69                     | 0.56              |
| 58:B1:247:PRO:HA   | 58:B1:250:ARG:HG3   | 1.87                     | 0.56              |
| 31:f:44:HIS:HA     | 31:f:49:LEU:HG      | 1.87                     | 0.56              |
| 39:o:52:SER:OG     | 39:o:53:THR:N       | 2.39                     | 0.56              |
| 51:1:359:G:C2'     | 51:1:360:U:H5'      | 2.36                     | 0.56              |
| 51:1:877:A:N1      | 51:1:899:A:H2'      | 2.20                     | 0.56              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 51:1:1485:U:H2'     | 51:1:1486:U:C6     | 2.41                     | 0.56              |
| 51:1:1678:A:H2'     | 51:1:1679:A:H5'    | 1.86                     | 0.56              |
| 58:B1:160:LEU:HD22  | 58:B1:164:GLN:HB3  | 1.86                     | 0.56              |
| 58:B1:1167:LYS:HZ2  | 58:B1:1170:LYS:HB2 | 1.71                     | 0.56              |
| 64:6:52:G:H2'       | 64:6:53:G:H8       | 1.69                     | 0.56              |
| 27:b:250:GLN:NE2    | 27:b:251:THR:O     | 2.38                     | 0.56              |
| 51:1:780:G:H21      | 51:1:783:A:H62     | 1.54                     | 0.56              |
| 51:1:1590:A:O2'     | 51:1:1591:A:H5'    | 2.05                     | 0.56              |
| 59:B2:13:LYS:HB2    | 59:B2:1180:MET:HE2 | 1.86                     | 0.56              |
| 7:G:91:VAL:HG22     | 7:G:150:ILE:HD11   | 1.88                     | 0.56              |
| 11:K:2:ARG:NH1      | 53:3:738:C:OP1     | 2.39                     | 0.56              |
| 11:K:12:PRO:HB2     | 11:K:44:ARG:HH21   | 1.70                     | 0.56              |
| 14:N:35:GLU:HA      | 14:N:39:GLY:HA3    | 1.86                     | 0.56              |
| 16:P:92:ARG:NH2     | 16:P:111:ASP:OD1   | 2.38                     | 0.56              |
| 38:n:2:ARG:HA       | 38:n:5:LYS:HD3     | 1.88                     | 0.56              |
| 50:z:15:ARG:HE      | 50:z:52:PHE:HE2    | 1.53                     | 0.56              |
| 51:1:296:U:H2'      | 51:1:297:G:C8      | 2.41                     | 0.56              |
| 51:1:1120:G:O2'     | 51:1:1121:C:H5'    | 2.05                     | 0.56              |
| 51:1:1410:G:H2'     | 51:1:1411:U:C6     | 2.41                     | 0.56              |
| 51:1:2395:C:H42     | 51:1:2421:G:H1     | 1.54                     | 0.56              |
| 53:3:159:G:N2       | 53:3:162:A:OP2     | 2.34                     | 0.56              |
| 58:B1:1046:ILE:HD12 | 58:B1:1059:LEU:HB3 | 1.86                     | 0.56              |
| 59:B2:1070:HIS:NE2  | 59:B2:1114:GLU:OE1 | 2.36                     | 0.56              |
| 31:f:40:VAL:O       | 31:f:54:ARG:NH2    | 2.38                     | 0.56              |
| 31:f:151:ARG:HB3    | 31:f:161:VAL:HG23  | 1.86                     | 0.56              |
| 49:y:49:ASP:OD1     | 49:y:52:ARG:NH2    | 2.39                     | 0.56              |
| 51:1:118:A:OP2      | 51:1:119:A:H5''    | 2.06                     | 0.56              |
| 51:1:720:U:H2'      | 51:1:721:A:C8      | 2.41                     | 0.56              |
| 51:1:1541:C:O2'     | 51:1:1542:U:H5'    | 2.06                     | 0.56              |
| 51:1:2457:U:O2'     | 51:1:2458:G:H5'    | 2.05                     | 0.56              |
| 51:1:2510:C:C4      | 51:1:2511:U:C4     | 2.93                     | 0.56              |
| 58:B1:39:LYS:O      | 58:B1:273:ILE:HG21 | 2.06                     | 0.56              |
| 58:B1:1166:GLY:HA3  | 58:B1:1174:ARG:HB2 | 1.88                     | 0.56              |
| 63:5:37:A:H3'       | 63:5:38:A:H8       | 1.71                     | 0.56              |
| 7:G:58:LYS:O        | 7:G:62:ARG:NH1     | 2.38                     | 0.56              |
| 51:1:1182:G:H2'     | 51:1:1183:U:O4'    | 2.06                     | 0.56              |
| 51:1:1485:U:H2'     | 51:1:1486:U:H6     | 1.70                     | 0.56              |
| 51:1:1597:A:H5''    | 51:1:1598:A:H5'    | 1.87                     | 0.56              |
| 51:1:2637:U:C2'     | 51:1:2638:G:H5'    | 2.36                     | 0.56              |
| 58:B1:130:MET:HE2   | 58:B1:135:ILE:HG12 | 1.87                     | 0.56              |
| 58:B1:804:ALA:HA    | 58:B1:1259:GLN:HG3 | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:1:78:U:H2'     | 51:1:79:C:C6      | 2.40                     | 0.56              |
| 51:1:133:U:O2'    | 51:1:134:G:H5'    | 2.06                     | 0.56              |
| 51:1:288:U:H2'    | 51:1:289:G:H8     | 1.71                     | 0.56              |
| 51:1:1097:U:H2'   | 51:1:1098:A:O4'   | 2.06                     | 0.56              |
| 51:1:1772:A:H5'   | 51:1:1773:A:OP2   | 2.06                     | 0.56              |
| 51:1:1917:U:O2'   | 51:1:1918:A:H5'   | 2.05                     | 0.56              |
| 51:1:2626:C:H2'   | 51:1:2627:G:O4'   | 2.06                     | 0.56              |
| 65:0:29:ARG:HE    | 65:0:269:ALA:HB1  | 1.70                     | 0.56              |
| 10:J:44:ARG:NH2   | 10:J:70:MET:SD    | 2.78                     | 0.56              |
| 51:1:2114:A:C2    | 51:1:2167:U:H1'   | 2.41                     | 0.56              |
| 57:A1:29:GLU:HB3  | 57:A1:200:LYS:HG3 | 1.88                     | 0.56              |
| 49:y:28:LEU:HA    | 49:y:31:GLN:HB2   | 1.88                     | 0.55              |
| 51:1:340:A:H2'    | 51:1:341:C:O4'    | 2.06                     | 0.55              |
| 51:1:759:G:H2'    | 51:1:760:G:C8     | 2.41                     | 0.55              |
| 51:1:2584:U:C2'   | 51:1:2585:U:H5'   | 2.34                     | 0.55              |
| 53:3:158:G:N2     | 53:3:163:C:O2     | 2.36                     | 0.55              |
| 53:3:830:G:H1     | 53:3:856:C:H42    | 1.53                     | 0.55              |
| 4:D:9:VAL:HG22    | 51:1:1309:G:OP1   | 2.06                     | 0.55              |
| 19:S:26:LEU:HA    | 19:S:30:ILE:HD12  | 1.87                     | 0.55              |
| 51:1:155:A:H2'    | 51:1:156:A:C8     | 2.41                     | 0.55              |
| 51:1:172:A:H2'    | 51:1:173:A:C8     | 2.40                     | 0.55              |
| 51:1:825:A:O2'    | 51:1:826:U:H5'    | 2.06                     | 0.55              |
| 51:1:1086:A:H5'   | 51:1:1103:A:C2    | 2.41                     | 0.55              |
| 51:1:1697:G:H4'   | 51:1:1978:A:H5''  | 1.88                     | 0.55              |
| 53:3:503:C:H2'    | 53:3:504:C:C6     | 2.41                     | 0.55              |
| 41:q:90:ASP:N     | 41:q:90:ASP:OD1   | 2.37                     | 0.55              |
| 51:1:439:A:H2'    | 51:1:440:C:C6     | 2.42                     | 0.55              |
| 51:1:633:A:C2'    | 51:1:634:C:H5'    | 2.35                     | 0.55              |
| 51:1:655:A:H4'    | 51:1:656:G:C5'    | 2.30                     | 0.55              |
| 51:1:885:C:N4     | 51:1:886:A:H62    | 2.03                     | 0.55              |
| 51:1:1506:U:H2'   | 51:1:1507:C:C6    | 2.41                     | 0.55              |
| 53:3:49:U:H3      | 53:3:362:G:H1'    | 1.71                     | 0.55              |
| 58:B1:102:MET:HG2 | 58:B1:246:PRO:HG3 | 1.87                     | 0.55              |
| 65:0:514:GLN:HE22 | 65:0:591:LEU:HD23 | 1.72                     | 0.55              |
| 12:L:4:ARG:HB3    | 12:L:6:ILE:HG23   | 1.88                     | 0.55              |
| 19:S:52:ARG:O     | 19:S:58:ARG:NH1   | 2.39                     | 0.55              |
| 28:c:134:HIS:CE1  | 51:1:1675:C:C4    | 2.94                     | 0.55              |
| 37:m:27:SER:H     | 37:m:66:ARG:HH12  | 1.54                     | 0.55              |
| 51:1:613:A:H2'    | 51:1:613:A:N3     | 2.21                     | 0.55              |
| 59:B2:985:GLU:HB3 | 59:B2:988:LYS:HB2 | 1.89                     | 0.55              |
| 51:1:184:C:H2'    | 51:1:185:G:C8     | 2.41                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:1:543:G:H2'     | 51:1:544:C:C4'      | 2.37                     | 0.55              |
| 51:1:877:A:C2'     | 51:1:878:A:H5''     | 2.37                     | 0.55              |
| 51:1:1448:G:H2'    | 51:1:1449:G:C8      | 2.42                     | 0.55              |
| 51:1:2236:U:H2'    | 51:1:2237:G:H5'     | 1.88                     | 0.55              |
| 58:B1:799:ARG:HG2  | 58:B1:1325:PHE:HZ   | 1.72                     | 0.55              |
| 59:B2:103:VAL:HB   | 59:B2:114:VAL:HG11  | 1.89                     | 0.55              |
| 59:B2:839:VAL:HG12 | 59:B2:1049:ILE:HG12 | 1.87                     | 0.55              |
| 26:Z:44:ARG:NH1    | 53:3:722:G:OP2      | 2.39                     | 0.55              |
| 27:b:216:ARG:NH2   | 51:1:781:A:OP1      | 2.38                     | 0.55              |
| 28:c:18:ASP:OD1    | 28:c:18:ASP:N       | 2.36                     | 0.55              |
| 51:1:296:U:H2'     | 51:1:297:G:H8       | 1.71                     | 0.55              |
| 51:1:1389:G:O2'    | 51:1:1390:U:H5'     | 2.07                     | 0.55              |
| 51:1:2488:G:O2'    | 51:1:2489:U:H5'     | 2.07                     | 0.55              |
| 51:1:2743:U:C3'    | 51:1:2744:G:H5''    | 2.37                     | 0.55              |
| 51:1:2845:U:H2'    | 51:1:2846:G:C8      | 2.42                     | 0.55              |
| 58:B1:833:GLU:HB2  | 58:B1:1242:ARG:NH1  | 2.22                     | 0.55              |
| 51:1:112:U:C2'     | 51:1:113:U:H5'      | 2.37                     | 0.55              |
| 51:1:359:G:H2'     | 51:1:360:U:O4'      | 2.07                     | 0.55              |
| 51:1:392:U:H2'     | 51:1:393:C:C6       | 2.42                     | 0.55              |
| 51:1:461:C:H2'     | 51:1:462:C:C6       | 2.41                     | 0.55              |
| 35:k:76:VAL:H      | 40:p:72:VAL:HG22    | 1.71                     | 0.55              |
| 43:s:98:LYS:HD3    | 51:1:2012:G:OP1     | 2.06                     | 0.55              |
| 49:y:19:LEU:O      | 49:y:23:ARG:N       | 2.35                     | 0.55              |
| 51:1:1048:A:H2'    | 51:1:1049:C:H5'     | 1.88                     | 0.55              |
| 51:1:1601:G:C2'    | 51:1:1602:U:H5'     | 2.37                     | 0.55              |
| 51:1:1909:C:H2'    | 51:1:1910:G:C8      | 2.41                     | 0.55              |
| 51:1:1948:G:H21    | 53:3:1418:A:H2      | 1.49                     | 0.55              |
| 51:1:2114:A:C8     | 51:1:2115:G:H1'     | 2.42                     | 0.55              |
| 53:3:202:G:H21     | 53:3:466:A:H61      | 1.53                     | 0.55              |
| 53:3:1040:U:H2'    | 53:3:1041:G:C8      | 2.42                     | 0.55              |
| 7:G:19:THR:HA      | 7:G:37:VAL:HA       | 1.88                     | 0.55              |
| 16:P:63:GLN:HG3    | 16:P:98:ALA:HB2     | 1.88                     | 0.55              |
| 51:1:279:A:N6      | 51:1:361:G:H1'      | 2.21                     | 0.55              |
| 51:1:1386:C:H2'    | 51:1:1387:A:C8      | 2.41                     | 0.55              |
| 51:1:2195:U:O2'    | 51:1:2196:C:H5'     | 2.06                     | 0.55              |
| 51:1:2217:G:O2'    | 51:1:2218:G:H5'     | 2.06                     | 0.55              |
| 51:1:2533:U:C2'    | 51:1:2534:A:H5'     | 2.36                     | 0.55              |
| 59:B2:917:SER:O    | 59:B2:919:ARG:HG3   | 2.07                     | 0.55              |
| 57:A1:47:LEU:HD23  | 57:A1:51:MET:HG3    | 1.89                     | 0.55              |
| 58:B1:58:CYS:SG    | 58:B1:59:ALA:N      | 2.80                     | 0.55              |
| 36:l:89:VAL:HG23   | 36:l:121:THR:HG23   | 1.88                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:1:1745:A:O2'    | 51:1:1746:A:H5'     | 2.07                     | 0.54              |
| 51:1:2345:G:H5'    | 51:1:2347:C:H5'     | 1.89                     | 0.54              |
| 51:1:2827:C:O2'    | 51:1:2828:G:H5'     | 2.07                     | 0.54              |
| 53:3:923:A:N6      | 53:3:1392:G:O6      | 2.40                     | 0.54              |
| 64:6:11:A:H2'      | 64:6:12:G:H8        | 1.72                     | 0.54              |
| 8:H:39:ARG:NH1     | 8:H:54:ILE:O        | 2.39                     | 0.54              |
| 12:L:73:GLU:HG2    | 12:L:90:VAL:HG22    | 1.89                     | 0.54              |
| 30:e:23:SER:HB3    | 30:e:26:GLN:HB2     | 1.88                     | 0.54              |
| 33:i:10:LEU:HA     | 51:1:1061:U:C2      | 2.42                     | 0.54              |
| 51:1:317:G:H2'     | 51:1:318:C:C6       | 2.42                     | 0.54              |
| 51:1:1005:C:H6     | 51:1:1005:C:O5'     | 1.90                     | 0.54              |
| 51:1:1545:A:H2'    | 51:1:1546:G:O4'     | 2.06                     | 0.54              |
| 53:3:927:G:O2'     | 53:3:1503:A:N7      | 2.38                     | 0.54              |
| 58:B1:144:TYR:HE1  | 58:B1:162:GLU:CD    | 2.14                     | 0.54              |
| 58:B1:145:VAL:HG23 | 58:B1:159:ILE:HG22  | 1.89                     | 0.54              |
| 58:B1:508:LEU:HD22 | 59:B2:1101:LEU:HD21 | 1.88                     | 0.54              |
| 58:B1:759:ILE:HG23 | 58:B1:771:GLN:HB3   | 1.89                     | 0.54              |
| 7:G:138:ARG:NH1    | 7:G:141:GLU:OE2     | 2.40                     | 0.54              |
| 51:1:622:G:HO2'    | 51:1:623:C:H5'      | 1.72                     | 0.54              |
| 51:1:1288:G:C6     | 51:1:1327:A:C2      | 2.96                     | 0.54              |
| 51:1:1310:G:O2'    | 51:1:1311:G:H5'     | 2.06                     | 0.54              |
| 53:3:1036:A:H2'    | 53:3:1037:C:H5'     | 1.88                     | 0.54              |
| 59:B2:29:SER:O     | 59:B2:33:ASP:HB2    | 2.07                     | 0.54              |
| 59:B2:684:ASN:OD1  | 59:B2:687:ARG:NH2   | 2.41                     | 0.54              |
| 64:6:9:G:C2        | 64:6:45:G:O6        | 2.60                     | 0.54              |
| 7:G:53:LEU:HD21    | 7:G:215:ALA:HB1     | 1.88                     | 0.54              |
| 12:L:113:LYS:O     | 53:3:1239:A:O2'     | 2.23                     | 0.54              |
| 16:P:86:LYS:HG3    | 16:P:114:PRO:HD3    | 1.89                     | 0.54              |
| 25:Y:47:GLN:NE2    | 25:Y:51:ASN:OD1     | 2.40                     | 0.54              |
| 29:d:84:THR:HG21   | 51:1:586:A:H5'      | 1.87                     | 0.54              |
| 37:m:64:TRP:HB2    | 37:m:104:GLU:HB2    | 1.89                     | 0.54              |
| 51:1:1297:C:H2'    | 51:1:1298:C:C6      | 2.43                     | 0.54              |
| 51:1:1670:C:O5'    | 51:1:1670:C:H6      | 1.90                     | 0.54              |
| 51:1:1748:C:H2'    | 51:1:1749:A:H8      | 1.73                     | 0.54              |
| 51:1:2091:C:H5     | 51:1:2092:U:HO2'    | 1.53                     | 0.54              |
| 51:1:2734:A:C2'    | 51:1:2735:G:H5'     | 2.38                     | 0.54              |
| 51:1:2850:A:N1     | 51:1:2869:G:H4'     | 2.21                     | 0.54              |
| 59:B2:360:LEU:HD13 | 59:B2:378:ARG:HH11  | 1.72                     | 0.54              |
| 51:1:128:C:H2'     | 51:1:129:C:H6       | 1.70                     | 0.54              |
| 51:1:268:C:H2'     | 51:1:269:C:H6       | 1.73                     | 0.54              |
| 51:1:1014:A:H2'    | 51:1:1015:U:C6      | 2.43                     | 0.54              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 52:2:40:U:N3        | 52:2:44:G:OP2       | 2.40                     | 0.54              |
| 57:A2:29:GLU:HG3    | 57:A2:200:LYS:HG3   | 1.88                     | 0.54              |
| 58:B1:1155:ILE:HG13 | 58:B1:1210:ILE:HB   | 1.89                     | 0.54              |
| 35:k:70:ARG:HG2     | 35:k:76:VAL:HG12    | 1.88                     | 0.54              |
| 38:n:35:LYS:NZ      | 38:n:100:CYS:SG     | 2.81                     | 0.54              |
| 51:1:472:A:H2'      | 51:1:473:G:H5'      | 1.90                     | 0.54              |
| 51:1:1091:G:H2'     | 51:1:1092:C:C6      | 2.43                     | 0.54              |
| 51:1:2545:G:O2'     | 51:1:2546:U:H5'     | 2.07                     | 0.54              |
| 59:B2:633:LEU:HD13  | 59:B2:644:LEU:HD23  | 1.89                     | 0.54              |
| 10:J:23:THR:HA      | 10:J:28:ARG:HA      | 1.88                     | 0.54              |
| 21:U:69:ASP:OD1     | 21:U:69:ASP:N       | 2.38                     | 0.54              |
| 29:d:76:PRO:HD2     | 51:1:673:C:H5''     | 1.89                     | 0.54              |
| 44:t:54:GLU:HB3     | 44:t:88:LYS:HE3     | 1.90                     | 0.54              |
| 51:1:682:G:N2       | 51:1:796:C:O2       | 2.41                     | 0.54              |
| 51:1:876:C:H2'      | 51:1:877:A:O4'      | 2.08                     | 0.54              |
| 51:1:1530:G:H22     | 51:1:1542:U:H1'     | 1.73                     | 0.54              |
| 58:B1:800:LEU:HB3   | 58:B1:920:ALA:HB1   | 1.89                     | 0.54              |
| 58:B1:1175:LEU:HD22 | 58:B1:1190:ILE:HD11 | 1.88                     | 0.54              |
| 59:B2:243:PRO:HB2   | 59:B2:274:ILE:HG23  | 1.90                     | 0.54              |
| 9:I:55:ARG:O        | 9:I:59:LYS:N        | 2.41                     | 0.54              |
| 34:j:38:GLY:HA3     | 34:j:50:THR:HG23    | 1.90                     | 0.54              |
| 51:1:143:C:H2'      | 51:1:144:A:H8       | 1.72                     | 0.54              |
| 51:1:923:G:O2'      | 51:1:924:G:H5'      | 2.07                     | 0.54              |
| 51:1:1856:U:H2'     | 51:1:1857:G:O4'     | 2.08                     | 0.54              |
| 51:1:2092:U:C5      | 51:1:2199:A:H2      | 2.25                     | 0.54              |
| 51:1:2328:A:H8      | 51:1:2328:A:O5'     | 1.90                     | 0.54              |
| 51:1:2742:G:O2'     | 51:1:2743:U:H5'     | 2.08                     | 0.54              |
| 58:B1:746:LEU:HG    | 58:B1:758:PRO:HG3   | 1.90                     | 0.54              |
| 58:B1:814:CYS:SG    | 58:B1:883:ARG:NH2   | 2.81                     | 0.54              |
| 59:B2:811:ASN:HA    | 59:B2:815:SER:HB2   | 1.90                     | 0.54              |
| 7:G:86:CYS:SG       | 7:G:87:ASP:N        | 2.74                     | 0.54              |
| 19:S:84:ARG:NH2     | 53:3:1059:C:O3'     | 2.40                     | 0.54              |
| 20:T:48:ASP:OD1     | 53:3:667:G:O2'      | 2.25                     | 0.54              |
| 25:Y:60:GLN:HA      | 25:Y:63:LYS:HB3     | 1.89                     | 0.54              |
| 29:d:76:PRO:HA      | 29:d:82:GLY:HA3     | 1.90                     | 0.54              |
| 49:y:15:ASN:O       | 49:y:19:LEU:N       | 2.41                     | 0.54              |
| 51:1:141:G:H3'      | 51:1:142:A:O4'      | 2.07                     | 0.54              |
| 51:1:1511:G:H2'     | 51:1:1512:C:H6      | 1.73                     | 0.54              |
| 51:1:2123:G:H2'     | 51:1:2124:G:H8      | 1.73                     | 0.54              |
| 51:1:2190:G:O2'     | 51:1:2191:A:H5'     | 2.08                     | 0.54              |
| 58:B1:30:ILE:HG21   | 58:B1:241:VAL:O     | 2.08                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:P:15:VAL:HG12   | 16:P:76:TYR:HB3    | 1.90                     | 0.54              |
| 27:b:227:VAL:HG11  | 51:1:784:G:N1      | 2.23                     | 0.54              |
| 31:f:103:ASN:ND2   | 31:f:113:ASP:OD1   | 2.41                     | 0.54              |
| 47:w:55:LEU:HD12   | 47:w:76:ILE:HD12   | 1.90                     | 0.54              |
| 51:1:2631:G:O2'    | 51:1:2632:A:H5'    | 2.08                     | 0.54              |
| 53:3:505:G:H5''    | 53:3:534:U:H2'     | 1.89                     | 0.54              |
| 58:B1:39:LYS:O     | 58:B1:273:ILE:HG23 | 2.08                     | 0.54              |
| 65:0:17:ALA:HB2    | 65:0:112:VAL:HB    | 1.89                     | 0.54              |
| 7:G:126:ASP:OD1    | 7:G:126:ASP:N      | 2.41                     | 0.53              |
| 51:1:8:C:H2'       | 51:1:9:G:H8        | 1.73                     | 0.53              |
| 51:1:341:C:O2'     | 51:1:342:A:H5'     | 2.08                     | 0.53              |
| 51:1:358:U:H2'     | 51:1:359:G:H8      | 1.72                     | 0.53              |
| 51:1:757:G:H2'     | 51:1:758:C:C5'     | 2.35                     | 0.53              |
| 51:1:1599:U:H2'    | 51:1:1600:C:C6     | 2.43                     | 0.53              |
| 53:3:458:U:H3      | 53:3:474:G:H1      | 1.56                     | 0.53              |
| 57:A2:28:LEU:HD22  | 57:A2:201:LEU:HD23 | 1.90                     | 0.53              |
| 58:B1:785:ASP:O    | 58:B1:789:LYS:HB2  | 2.08                     | 0.53              |
| 17:Q:8:ARG:NH2     | 53:3:880:C:OP1     | 2.36                     | 0.53              |
| 51:1:176:A:O2'     | 51:1:177:G:H5'     | 2.08                     | 0.53              |
| 51:1:441:U:O2'     | 51:1:442:G:H5'     | 2.08                     | 0.53              |
| 51:1:543:G:C2'     | 51:1:544:C:H5''    | 2.37                     | 0.53              |
| 51:1:1601:G:O2'    | 51:1:1602:U:H5'    | 2.08                     | 0.53              |
| 51:1:2850:A:C2     | 51:1:2869:G:H4'    | 2.44                     | 0.53              |
| 53:3:1023:U:H2'    | 53:3:1024:G:C8     | 2.43                     | 0.53              |
| 58:B1:111:THR:HG22 | 58:B1:300:GLN:NE2  | 2.23                     | 0.53              |
| 64:6:25:C:H42      | 64:6:45:G:H22      | 1.56                     | 0.53              |
| 1:A:35:ASP:OD1     | 18:R:2:ARG:NH1     | 2.42                     | 0.53              |
| 3:C:20:TYR:OH      | 51:1:2348:U:H5'    | 2.08                     | 0.53              |
| 12:L:77:ARG:NH2    | 53:3:1381:U:O2     | 2.41                     | 0.53              |
| 51:1:613:A:H5''    | 51:1:614:A:N7      | 2.22                     | 0.53              |
| 58:B1:78:LEU:O     | 58:B1:78:LEU:HD13  | 2.08                     | 0.53              |
| 8:H:71:ARG:HB3     | 8:H:74:ILE:HD13    | 1.89                     | 0.53              |
| 10:J:104:ILE:O     | 10:J:111:ARG:NH1   | 2.41                     | 0.53              |
| 11:K:23:GLU:HA     | 11:K:26:THR:HG22   | 1.90                     | 0.53              |
| 30:e:21:TYR:OH     | 30:e:164:GLU:OE1   | 2.26                     | 0.53              |
| 51:1:53:A:H2'      | 51:1:54:G:H5'      | 1.89                     | 0.53              |
| 51:1:1083:U:H2'    | 51:1:1084:A:H3'    | 1.89                     | 0.53              |
| 51:1:1913:A:N7     | 53:3:1494:G:H4'    | 2.22                     | 0.53              |
| 51:1:2092:U:C5     | 51:1:2199:A:C2     | 2.97                     | 0.53              |
| 51:1:2644:G:O2'    | 51:1:2645:G:H5'    | 2.09                     | 0.53              |
| 57:A1:16:ILE:HG23  | 57:A1:26:VAL:HG22  | 1.91                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 59:B2:1117:LEU:HD12 | 59:B2:1195:ILE:HG12 | 1.90                     | 0.53              |
| 36:l:80:SER:HB3     | 36:l:114:GLY:HA3    | 1.90                     | 0.53              |
| 51:1:40:U:H2'       | 51:1:41:C:C6        | 2.43                     | 0.53              |
| 51:1:44:A:O2'       | 51:1:45:G:H5'       | 2.08                     | 0.53              |
| 51:1:402:A:C2'      | 51:1:403:U:H5'      | 2.38                     | 0.53              |
| 51:1:1560:G:H2'     | 51:1:1560:G:N3      | 2.24                     | 0.53              |
| 51:1:2617:U:H2'     | 51:1:2618:G:H5'     | 1.91                     | 0.53              |
| 53:3:1077:G:N2      | 53:3:1080:A:OP2     | 2.40                     | 0.53              |
| 13:M:92:PRO:O       | 13:M:116:ARG:NH2    | 2.42                     | 0.53              |
| 33:i:53:PRO:HD2     | 33:i:77:VAL:HG11    | 1.91                     | 0.53              |
| 36:l:20:GLY:HA2     | 36:l:28:GLY:HA2     | 1.90                     | 0.53              |
| 39:o:31:THR:HG23    | 39:o:34:HIS:H       | 1.73                     | 0.53              |
| 39:o:69:ASP:N       | 39:o:69:ASP:OD1     | 2.36                     | 0.53              |
| 51:1:481:G:H1'      | 51:1:506:G:H21      | 1.71                     | 0.53              |
| 51:1:925:A:O2'      | 51:1:926:G:H5'      | 2.08                     | 0.53              |
| 51:1:995:C:H6       | 51:1:995:C:H5'      | 1.74                     | 0.53              |
| 51:1:1662:U:H2'     | 51:1:1663:G:O4'     | 2.09                     | 0.53              |
| 17:Q:64:SER:OG      | 17:Q:65:TYR:N       | 2.41                     | 0.53              |
| 48:x:29:LEU:HD12    | 51:1:2230:G:H5''    | 1.90                     | 0.53              |
| 51:1:53:A:C2'       | 51:1:54:G:H5'       | 2.39                     | 0.53              |
| 51:1:611:C:H2'      | 51:1:612:G:O4'      | 2.09                     | 0.53              |
| 51:1:820:A:O2'      | 51:1:821:A:H5'      | 2.08                     | 0.53              |
| 51:1:878:A:H2'      | 51:1:879:G:O4'      | 2.09                     | 0.53              |
| 51:1:973:A:H5'      | 51:1:1188:U:H1'     | 1.90                     | 0.53              |
| 51:1:1068:G:N2      | 51:1:1096:A:H1'     | 2.23                     | 0.53              |
| 51:1:1528:A:C2'     | 51:1:1529:G:H5'     | 2.38                     | 0.53              |
| 57:A1:100:LEU:HD21  | 57:A1:121:VAL:HG11  | 1.90                     | 0.53              |
| 8:H:30:ASP:N        | 8:H:30:ASP:OD1      | 2.41                     | 0.53              |
| 40:p:105:LYS:O      | 40:p:108:ARG:NH2    | 2.42                     | 0.53              |
| 51:1:282:A:H2'      | 51:1:283:G:C8       | 2.42                     | 0.53              |
| 51:1:1171:G:H2'     | 51:1:1172:C:C4'     | 2.38                     | 0.53              |
| 51:1:1409:U:H2'     | 51:1:1410:G:C8      | 2.44                     | 0.53              |
| 51:1:1678:A:H2'     | 51:1:1679:A:C5'     | 2.38                     | 0.53              |
| 51:1:1917:U:C2'     | 51:1:1918:A:H5'     | 2.39                     | 0.53              |
| 53:3:1023:U:H2'     | 53:3:1024:G:H8      | 1.74                     | 0.53              |
| 9:I:154:VAL:HA      | 9:I:157:ALA:HB3     | 1.91                     | 0.53              |
| 14:N:115:VAL:HG23   | 53:3:1367:C:H5''    | 1.91                     | 0.53              |
| 40:p:28:LYS:HB3     | 40:p:39:LEU:HD21    | 1.91                     | 0.53              |
| 51:1:21:A:O2'       | 51:1:22:C:H5'       | 2.08                     | 0.53              |
| 51:1:140:C:H2'      | 51:1:141:G:H5'      | 1.90                     | 0.53              |
| 51:1:268:C:H2'      | 51:1:269:C:C6       | 2.44                     | 0.53              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:1:894:U:O2'     | 51:1:895:U:H5'      | 2.09                     | 0.53              |
| 51:1:1063:G:N1     | 51:1:1075:C:N4      | 2.53                     | 0.53              |
| 51:1:2425:A:H4'    | 51:1:2426:A:H5''    | 1.91                     | 0.53              |
| 51:1:2758:A:H2'    | 51:1:2759:G:C5'     | 2.39                     | 0.53              |
| 57:A2:100:LEU:HD23 | 57:A2:115:ILE:HG21  | 1.89                     | 0.53              |
| 58:B1:770:LEU:CD1  | 59:B2:618:GLN:HG3   | 2.37                     | 0.53              |
| 58:B1:975:ILE:HD11 | 58:B1:1003:LEU:HD11 | 1.91                     | 0.53              |
| 59:B2:628:HIS:HB3  | 59:B2:647:ARG:HH21  | 1.74                     | 0.53              |
| 7:G:61:SER:OG      | 7:G:62:ARG:NH1      | 2.42                     | 0.53              |
| 31:f:7:PRO:O       | 31:f:68:ARG:NH2     | 2.38                     | 0.53              |
| 34:j:2:LYS:HA      | 51:1:995:C:N3       | 2.23                     | 0.53              |
| 51:1:1530:G:N2     | 51:1:1542:U:H1'     | 2.23                     | 0.53              |
| 51:1:1782:U:H2'    | 51:1:1783:A:H5''    | 1.90                     | 0.53              |
| 51:1:2092:U:C4'    | 51:1:2093:G:H5''    | 2.37                     | 0.53              |
| 51:1:2297:A:N1     | 51:1:2321:U:C5      | 2.75                     | 0.53              |
| 51:1:2747:G:O6     | 51:1:2754:U:H2'     | 2.09                     | 0.53              |
| 53:3:1244:G:H1     | 53:3:1293:C:H42     | 1.57                     | 0.53              |
| 8:H:133:MET:HE3    | 8:H:167:TYR:HB2     | 1.91                     | 0.52              |
| 25:Y:66:ILE:HG21   | 25:Y:70:LYS:HB3     | 1.91                     | 0.52              |
| 39:o:40:ILE:HD12   | 39:o:44:GLY:HA2     | 1.91                     | 0.52              |
| 42:r:4:VAL:HG12    | 42:r:13:ARG:HA      | 1.91                     | 0.52              |
| 50:z:36:GLU:O      | 50:z:37:ARG:NH1     | 2.42                     | 0.52              |
| 51:1:57:C:H2'      | 51:1:58:G:O4'       | 2.08                     | 0.52              |
| 51:1:1574:C:H2'    | 51:1:1575:C:H6      | 1.74                     | 0.52              |
| 51:1:1827:U:H2'    | 51:1:1828:G:H5'     | 1.90                     | 0.52              |
| 51:1:2194:U:H2'    | 51:1:2195:U:C6      | 2.44                     | 0.52              |
| 51:1:2204:G:H2'    | 51:1:2205:A:C8      | 2.44                     | 0.52              |
| 58:B1:68:TYR:CA    | 58:B1:75:TYR:HE2    | 2.22                     | 0.52              |
| 27:b:92:LEU:HD11   | 27:b:100:ARG:HB3    | 1.91                     | 0.52              |
| 51:1:1278:C:O2'    | 51:1:1279:G:H5'     | 2.09                     | 0.52              |
| 53:3:1266:G:N2     | 53:3:1269:A:OP2     | 2.29                     | 0.52              |
| 57:A2:43:LEU:HD13  | 57:A2:217:ILE:HD11  | 1.90                     | 0.52              |
| 64:6:43:A:H2'      | 64:6:44:A:C8        | 2.44                     | 0.52              |
| 30:e:91:ARG:NH2    | 52:2:43:C:O2        | 2.36                     | 0.52              |
| 51:1:519:U:H2'     | 51:1:520:G:H8       | 1.75                     | 0.52              |
| 51:1:752:A:H62     | 51:1:2609:U:H3      | 1.56                     | 0.52              |
| 51:1:1111:A:H2'    | 51:1:1112:G:H4'     | 1.90                     | 0.52              |
| 53:3:203:G:N2      | 53:3:204:G:O6       | 2.43                     | 0.52              |
| 58:B1:633:ALA:HB2  | 59:B2:808:ASN:N     | 2.19                     | 0.52              |
| 51:1:1794:A:O2'    | 51:1:1795:C:H5'     | 2.10                     | 0.52              |
| 51:1:2463:C:O2'    | 51:1:2464:G:H5'     | 2.10                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:1:2758:A:C2'   | 51:1:2759:G:H5'    | 2.40                     | 0.52              |
| 51:1:2762:C:C2'   | 51:1:2763:G:H5'    | 2.39                     | 0.52              |
| 58:B1:390:LEU:N   | 58:B1:390:LEU:CD1  | 2.73                     | 0.52              |
| 1:A:9:TYR:OH      | 30:e:101:ARG:NH2   | 2.41                     | 0.52              |
| 17:Q:36:VAL:HG21  | 17:Q:73:LEU:HB3    | 1.91                     | 0.52              |
| 51:1:870:U:O2'    | 51:1:871:U:H5'     | 2.10                     | 0.52              |
| 51:1:1310:G:H2'   | 51:1:1311:G:C5'    | 2.38                     | 0.52              |
| 51:1:2670:A:H2'   | 51:1:2671:G:H8     | 1.75                     | 0.52              |
| 57:A1:205:MET:HE3 | 57:A1:213:PRO:HB3  | 1.90                     | 0.52              |
| 58:B1:112:ALA:HA  | 58:B1:238:ILE:HA   | 1.91                     | 0.52              |
| 17:Q:49:ARG:NH1   | 17:Q:88:ASP:OD2    | 2.42                     | 0.52              |
| 51:1:251:A:H2'    | 51:1:252:G:O4'     | 2.10                     | 0.52              |
| 51:1:597:G:H2'    | 51:1:598:U:C6      | 2.45                     | 0.52              |
| 51:1:2102:G:H2'   | 51:1:2103:C:O4'    | 2.09                     | 0.52              |
| 51:1:2707:U:H2'   | 51:1:2708:G:C8     | 2.44                     | 0.52              |
| 59:B2:125:GLY:HA2 | 59:B2:499:SER:HB2  | 1.92                     | 0.52              |
| 26:Z:28:LEU:HA    | 26:Z:31:VAL:HG12   | 1.90                     | 0.52              |
| 27:b:257:ARG:NH2  | 27:b:262:THR:OG1   | 2.42                     | 0.52              |
| 42:r:51:VAL:HG22  | 42:r:52:PRO:HD2    | 1.92                     | 0.52              |
| 42:r:75:VAL:HG23  | 42:r:86:GLN:HG2    | 1.90                     | 0.52              |
| 46:v:77:VAL:HG23  | 46:v:89:ILE:HG12   | 1.92                     | 0.52              |
| 51:1:213:A:O2'    | 51:1:214:G:H5'     | 2.09                     | 0.52              |
| 51:1:2236:U:C2'   | 51:1:2237:G:H5'    | 2.39                     | 0.52              |
| 51:1:2611:C:O2    | 51:1:2611:C:C2'    | 2.58                     | 0.52              |
| 51:1:2670:A:H2'   | 51:1:2671:G:C8     | 2.45                     | 0.52              |
| 58:B1:832:LYS:HB3 | 58:B1:1242:ARG:NH1 | 2.24                     | 0.52              |
| 7:G:14:HIS:HB3    | 7:G:42:LEU:HD21    | 1.91                     | 0.52              |
| 7:G:102:ASN:ND2   | 53:3:1073:U:O2     | 2.39                     | 0.52              |
| 8:H:107:LYS:HB3   | 8:H:110:LEU:HD23   | 1.92                     | 0.52              |
| 23:W:52:ARG:NH2   | 53:3:835:U:OP1     | 2.42                     | 0.52              |
| 28:c:23:PRO:HB3   | 51:1:2682:A:N3     | 2.24                     | 0.52              |
| 51:1:215:G:C4'    | 51:1:216:A:H4'     | 2.39                     | 0.52              |
| 51:1:729:G:H5''   | 51:1:730:A:H5''    | 1.92                     | 0.52              |
| 51:1:784:G:C5'    | 51:1:785:G:OP1     | 2.54                     | 0.52              |
| 51:1:1503:A:C3'   | 51:1:1504:A:H5''   | 2.40                     | 0.52              |
| 51:1:1507:C:H2'   | 51:1:1508:A:C4'    | 2.40                     | 0.52              |
| 51:1:1534:U:H2'   | 51:1:1536:C:O4'    | 2.10                     | 0.52              |
| 51:1:1542:U:O2'   | 51:1:1543:G:H5'    | 2.09                     | 0.52              |
| 51:1:1558:C:O4'   | 51:1:1560:G:C8     | 2.62                     | 0.52              |
| 51:1:2216:G:H2'   | 51:1:2217:G:H8     | 1.74                     | 0.52              |
| 51:1:2625:G:O2'   | 51:1:2626:C:H5'    | 2.09                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:6:9:G:O4'       | 64:6:46:G:N3       | 2.42                     | 0.52              |
| 9:I:150:LYS:O      | 9:I:155:LYS:NZ     | 2.43                     | 0.52              |
| 10:J:152:VAL:HG21  | 13:M:98:LEU:HD13   | 1.91                     | 0.52              |
| 33:i:56:VAL:HB     | 33:i:68:PHE:HB2    | 1.92                     | 0.52              |
| 51:1:8:C:H2'       | 51:1:9:G:C8        | 2.45                     | 0.52              |
| 51:1:1403:A:H2'    | 51:1:1404:C:C6     | 2.45                     | 0.52              |
| 51:1:2570:G:C2'    | 51:1:2571:U:H5'    | 2.40                     | 0.52              |
| 51:1:2731:G:H2'    | 51:1:2732:G:C8     | 2.45                     | 0.52              |
| 58:B1:144:TYR:CE1  | 58:B1:162:GLU:CD   | 2.88                     | 0.52              |
| 35:k:42:THR:HG22   | 35:k:57:VAL:HG12   | 1.91                     | 0.52              |
| 51:1:1789:A:H2'    | 51:1:1790:C:O4'    | 2.09                     | 0.52              |
| 51:1:1878:G:O2'    | 51:1:1879:C:H5'    | 2.09                     | 0.52              |
| 51:1:2013:A:H5''   | 51:1:2013:A:C8     | 2.43                     | 0.52              |
| 58:B1:209:ASN:HA   | 58:B1:214:ARG:HH21 | 1.73                     | 0.52              |
| 59:B2:524:ILE:HG21 | 59:B2:708:VAL:HG13 | 1.92                     | 0.52              |
| 39:o:40:ILE:HG22   | 39:o:47:VAL:HG12   | 1.91                     | 0.51              |
| 51:1:208:C:O5'     | 51:1:208:C:H6      | 1.93                     | 0.51              |
| 51:1:1047:G:N2     | 51:1:1110:G:H2'    | 2.25                     | 0.51              |
| 51:1:1722:A:O2'    | 51:1:1723:G:H5'    | 2.10                     | 0.51              |
| 57:A2:140:ILE:HD12 | 57:A2:142:MET:HE3  | 1.91                     | 0.51              |
| 59:B2:786:GLY:N    | 59:B2:789:THR:OG1  | 2.41                     | 0.51              |
| 62:NG:161:SER:HA   | 62:NG:170:PRO:HA   | 1.92                     | 0.51              |
| 65:0:267:GLY:HA3   | 65:0:274:GLY:HA3   | 1.91                     | 0.51              |
| 45:u:73:ASN:ND2    | 45:u:80:ASP:OD2    | 2.43                     | 0.51              |
| 51:1:386:G:H3'     | 51:1:387:U:H5''    | 1.92                     | 0.51              |
| 51:1:723:C:O2'     | 51:1:724:U:H5'     | 2.09                     | 0.51              |
| 51:1:724:U:O2'     | 51:1:725:G:H5'     | 2.11                     | 0.51              |
| 51:1:1722:A:H62    | 51:1:1738:G:H1'    | 1.75                     | 0.51              |
| 51:1:2470:G:O2'    | 51:1:2471:A:H5'    | 2.10                     | 0.51              |
| 51:1:2529:G:H5''   | 51:1:2530:A:H5''   | 1.91                     | 0.51              |
| 58:B1:99:ARG:HA    | 58:B1:248:ASP:HB2  | 1.92                     | 0.51              |
| 58:B1:205:LEU:HG   | 58:B1:217:LEU:HB3  | 1.90                     | 0.51              |
| 65:0:674:THR:O     | 65:0:677:ARG:HG3   | 2.11                     | 0.51              |
| 14:N:89:TYR:HB3    | 14:N:93:LEU:HD21   | 1.92                     | 0.51              |
| 15:O:24:GLU:HA     | 15:O:27:GLU:HB2    | 1.93                     | 0.51              |
| 21:U:6:LEU:HD22    | 21:U:17:TYR:HB3    | 1.91                     | 0.51              |
| 23:W:71:ASP:N      | 23:W:71:ASP:OD1    | 2.44                     | 0.51              |
| 36:l:42:SER:HB2    | 51:1:672:C:H5      | 1.76                     | 0.51              |
| 43:s:67:ASP:OD1    | 43:s:67:ASP:N      | 2.39                     | 0.51              |
| 44:t:65:GLY:N      | 44:t:79:ASP:OD1    | 2.43                     | 0.51              |
| 51:1:1112:G:H2'    | 51:1:1113:U:O4'    | 2.10                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1:1338:G:H2'    | 51:1:1339:G:H8     | 1.74                     | 0.51              |
| 51:1:1923:U:H2'    | 51:1:1924:C:C6     | 2.45                     | 0.51              |
| 51:1:2651:C:O2'    | 51:1:2652:C:H5'    | 2.10                     | 0.51              |
| 53:3:202:G:H1      | 53:3:215:C:H42     | 1.57                     | 0.51              |
| 58:B1:215:LYS:HA   | 58:B1:218:THR:HG22 | 1.91                     | 0.51              |
| 3:C:7:LYS:HD3      | 51:1:2420:C:H5''   | 1.93                     | 0.51              |
| 35:k:31:ARG:NH2    | 51:1:2676:C:OP2    | 2.44                     | 0.51              |
| 51:1:49:A:O5'      | 51:1:51:G:H5'      | 2.09                     | 0.51              |
| 51:1:138:U:C5      | 51:1:139:U:H5      | 2.27                     | 0.51              |
| 51:1:355:U:H2'     | 51:1:356:G:C8      | 2.45                     | 0.51              |
| 51:1:2776:A:C6     | 51:1:2782:G:H1'    | 2.45                     | 0.51              |
| 65:0:632:ILE:HD11  | 65:0:654:ILE:HD12  | 1.91                     | 0.51              |
| 51:1:69:C:H2'      | 51:1:70:G:C8       | 2.46                     | 0.51              |
| 51:1:492:A:H2'     | 51:1:493:G:O4'     | 2.09                     | 0.51              |
| 51:1:736:C:H42     | 51:1:760:G:H1      | 1.59                     | 0.51              |
| 51:1:800:A:H4'     | 51:1:801:G:H3'     | 1.92                     | 0.51              |
| 58:B1:99:ARG:HG3   | 58:B1:99:ARG:HH11  | 1.73                     | 0.51              |
| 58:B1:972:LYS:HD2  | 58:B1:1004:ALA:HA  | 1.93                     | 0.51              |
| 59:B2:246:LEU:HB3  | 59:B2:269:ILE:HD13 | 1.91                     | 0.51              |
| 8:H:130:ARG:NH2    | 8:H:165:GLU:OE1    | 2.43                     | 0.51              |
| 8:H:175:HIS:ND1    | 53:3:1109:C:OP2    | 2.44                     | 0.51              |
| 10:J:23:THR:HG22   | 10:J:28:ARG:HB3    | 1.91                     | 0.51              |
| 10:J:106:ALA:O     | 10:J:111:ARG:NH2   | 2.43                     | 0.51              |
| 21:U:25:ARG:O      | 53:3:110:C:O2'     | 2.28                     | 0.51              |
| 51:1:286:U:H2'     | 51:1:287:G:H8      | 1.76                     | 0.51              |
| 51:1:1270:C:H5''   | 51:1:1271:G:H5''   | 1.93                     | 0.51              |
| 51:1:1678:A:C2'    | 51:1:1679:A:H5'    | 2.41                     | 0.51              |
| 51:1:1754:A:C6     | 51:1:1755:A:C6     | 2.98                     | 0.51              |
| 58:B1:111:THR:HG23 | 58:B1:300:GLN:NE2  | 2.24                     | 0.51              |
| 58:B1:201:LEU:HD12 | 58:B1:224:LEU:HD12 | 1.92                     | 0.51              |
| 51:1:2105:U:N3     | 51:1:2184:A:C2     | 2.78                     | 0.51              |
| 51:1:2618:G:H2'    | 51:1:2619:C:O4'    | 2.11                     | 0.51              |
| 53:3:494:G:H2'     | 53:3:496:A:H8      | 1.76                     | 0.51              |
| 65:0:647:SER:HA    | 65:0:652:VAL:HA    | 1.92                     | 0.51              |
| 2:B:2:VAL:HG23     | 51:1:2015:A:C6     | 2.46                     | 0.51              |
| 15:O:5:ARG:N       | 15:O:76:ILE:O      | 2.43                     | 0.51              |
| 17:Q:70:GLY:O      | 17:Q:107:LYS:NZ    | 2.44                     | 0.51              |
| 22:V:60:ILE:HA     | 22:V:74:LEU:HA     | 1.93                     | 0.51              |
| 27:b:50:THR:HG23   | 51:1:1813:G:H21    | 1.76                     | 0.51              |
| 51:1:291:G:O2'     | 51:1:292:U:H5'     | 2.11                     | 0.51              |
| 51:1:707:G:H2'     | 51:1:708:G:O4'     | 2.11                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1:1175:A:H3'    | 51:1:1176:U:C5'    | 2.37                     | 0.51              |
| 51:1:1266:G:O2'    | 51:1:2012:G:O6     | 2.25                     | 0.51              |
| 51:1:2285:C:O2'    | 51:1:2286:G:H5'    | 2.11                     | 0.51              |
| 58:B1:275:ARG:HH12 | 58:B1:278:ARG:NH1  | 2.09                     | 0.51              |
| 58:B1:375:GLU:HG2  | 59:B2:1245:ALA:O   | 2.10                     | 0.51              |
| 58:B1:437:PHE:HZ   | 58:B1:453:VAL:HG11 | 1.76                     | 0.51              |
| 60:W0:3:ARG:NH1    | 60:W0:55:GLU:OE2   | 2.40                     | 0.51              |
| 10:J:123:LEU:HD12  | 53:3:7:A:H2'       | 1.92                     | 0.51              |
| 35:k:75:SER:OG     | 40:p:72:VAL:O      | 2.26                     | 0.51              |
| 51:1:1415:U:H1'    | 51:1:1588:G:N2     | 2.26                     | 0.51              |
| 51:1:1441:G:H2'    | 51:1:1442:U:H6     | 1.71                     | 0.51              |
| 51:1:2525:G:N2     | 51:1:2539:C:C2     | 2.79                     | 0.51              |
| 53:3:780:A:N6      | 53:3:801:U:OP2     | 2.42                     | 0.51              |
| 59:B2:93:SER:HA    | 59:B2:128:PRO:HA   | 1.92                     | 0.51              |
| 27:b:92:LEU:HD21   | 27:b:100:ARG:HD3   | 1.93                     | 0.51              |
| 37:m:38:ARG:HB3    | 37:m:98:PRO:HD3    | 1.92                     | 0.51              |
| 51:1:630:G:H4'     | 51:1:640:C:H4'     | 1.93                     | 0.51              |
| 51:1:891:G:H2'     | 51:1:892:A:C8      | 2.46                     | 0.51              |
| 51:1:1930:G:C2'    | 51:1:1931:U:OP2    | 2.58                     | 0.51              |
| 58:B1:683:ILE:HD12 | 58:B1:754:ILE:HG21 | 1.92                     | 0.51              |
| 59:B2:400:VAL:HG11 | 59:B2:452:ARG:HD2  | 1.93                     | 0.51              |
| 28:c:176:ASP:OD1   | 28:c:176:ASP:N     | 2.44                     | 0.50              |
| 51:1:539:G:O2'     | 51:1:540:C:H5'     | 2.12                     | 0.50              |
| 51:1:1293:C:H2'    | 51:1:1294:U:C6     | 2.46                     | 0.50              |
| 51:1:2687:U:H2'    | 51:1:2688:G:O4'    | 2.11                     | 0.50              |
| 53:3:1538:C:O2'    | 53:3:1539:C:H5'    | 2.11                     | 0.50              |
| 58:B1:749:LYS:HB3  | 58:B1:755:ILE:HD11 | 1.94                     | 0.50              |
| 59:B2:714:VAL:HB   | 59:B2:787:PRO:HD2  | 1.92                     | 0.50              |
| 9:I:12:ARG:NH1     | 9:I:32:LYS:O       | 2.42                     | 0.50              |
| 15:O:29:ALA:O      | 15:O:33:GLY:N      | 2.42                     | 0.50              |
| 27:b:147:PRO:HG3   | 27:b:184:GLU:HG2   | 1.92                     | 0.50              |
| 27:b:207:ALA:HB2   | 51:1:1790:C:O2'    | 2.12                     | 0.50              |
| 38:n:49:GLU:O      | 38:n:53:THR:OG1    | 2.29                     | 0.50              |
| 48:x:64:ASP:N      | 48:x:64:ASP:OD1    | 2.43                     | 0.50              |
| 51:1:757:G:C2'     | 51:1:758:C:H5'     | 2.38                     | 0.50              |
| 51:1:2052:A:C2'    | 51:1:2053:G:H5'    | 2.41                     | 0.50              |
| 51:1:2555:U:O2     | 51:1:2555:U:O4'    | 2.29                     | 0.50              |
| 55:8:13:DT:OP2     | 58:B1:791:ALA:CB   | 2.59                     | 0.50              |
| 4:D:3:ARG:NH1      | 51:1:752:A:OP1     | 2.43                     | 0.50              |
| 11:K:42:TRP:HB2    | 11:K:59:TYR:HB2    | 1.93                     | 0.50              |
| 30:e:162:ASP:OD1   | 30:e:162:ASP:N     | 2.37                     | 0.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:1:145:C:H2'     | 51:1:146:A:C8       | 2.46                     | 0.50              |
| 51:1:386:G:H3'     | 51:1:387:U:C5'      | 2.41                     | 0.50              |
| 51:1:1388:G:O2'    | 51:1:1389:G:H5'     | 2.12                     | 0.50              |
| 51:1:1910:G:H1     | 51:1:1920:C:H42     | 1.58                     | 0.50              |
| 51:1:2248:C:H2'    | 51:1:2249:U:H5'     | 1.93                     | 0.50              |
| 53:3:113:G:N3      | 53:3:353:A:O2'      | 2.42                     | 0.50              |
| 58:B1:505:ASP:OD2  | 59:B2:812:PHE:HA    | 2.11                     | 0.50              |
| 58:B1:850:LYS:HB2  | 58:B1:857:LEU:HB2   | 1.91                     | 0.50              |
| 59:B2:255:ILE:HB   | 59:B2:263:VAL:HB    | 1.92                     | 0.50              |
| 11:K:46:GLN:HA     | 11:K:56:LYS:HB3     | 1.94                     | 0.50              |
| 30:e:135:ILE:HG23  | 30:e:140:ILE:HD11   | 1.93                     | 0.50              |
| 51:1:288:U:H2'     | 51:1:289:G:C8       | 2.47                     | 0.50              |
| 51:1:438:G:H2'     | 51:1:439:A:H8       | 1.76                     | 0.50              |
| 51:1:439:A:H2'     | 51:1:440:C:H6       | 1.75                     | 0.50              |
| 51:1:521:U:H2'     | 51:1:522:A:H8       | 1.73                     | 0.50              |
| 51:1:905:A:H2'     | 51:1:906:U:C5'      | 2.40                     | 0.50              |
| 51:1:2250:G:H8     | 51:1:2250:G:O5'     | 1.95                     | 0.50              |
| 51:1:2302:U:O2'    | 51:1:2303:G:H5'     | 2.12                     | 0.50              |
| 59:B2:400:VAL:HG21 | 59:B2:452:ARG:HE    | 1.76                     | 0.50              |
| 31:f:136:ASP:HB3   | 31:f:139:VAL:HG12   | 1.92                     | 0.50              |
| 51:1:187:G:C6      | 51:1:188:G:N7       | 2.80                     | 0.50              |
| 51:1:1676:A:H8     | 51:1:1676:A:O5'     | 1.95                     | 0.50              |
| 51:1:2286:G:H21    | 51:1:2287:A:N6      | 2.09                     | 0.50              |
| 51:1:2593:U:O2'    | 51:1:2594:C:H5'     | 2.11                     | 0.50              |
| 59:B2:974:ARG:HD2  | 59:B2:1014:LEU:HD21 | 1.92                     | 0.50              |
| 64:6:9:G:C2        | 64:6:45:G:C6        | 3.00                     | 0.50              |
| 64:6:9:G:O4'       | 64:6:46:G:C2        | 2.65                     | 0.50              |
| 4:D:14:ARG:NH1     | 51:1:1377:G:O3'     | 2.44                     | 0.50              |
| 20:T:2:LEU:HD22    | 20:T:34:GLN:HB2     | 1.92                     | 0.50              |
| 20:T:23:SER:OG     | 20:T:25:GLU:OE1     | 2.30                     | 0.50              |
| 27:b:56:GLY:HA2    | 27:b:212:TRP:HA     | 1.94                     | 0.50              |
| 28:c:161:MET:HE1   | 51:1:2050:C:O2      | 2.11                     | 0.50              |
| 51:1:197:A:H2      | 51:1:2434:A:N6      | 2.10                     | 0.50              |
| 51:1:673:C:H2'     | 51:1:674:G:C5'      | 2.41                     | 0.50              |
| 51:1:1161:C:H2'    | 51:1:1162:G:C8      | 2.44                     | 0.50              |
| 51:1:2888:C:H2'    | 51:1:2889:C:H6      | 1.77                     | 0.50              |
| 53:3:460:A:H2'     | 53:3:461:A:H8       | 1.75                     | 0.50              |
| 53:3:664:G:H22     | 53:3:741:G:H1       | 1.60                     | 0.50              |
| 63:5:34:G:H3'      | 63:5:35:A:H8        | 1.76                     | 0.50              |
| 1:A:35:ASP:OD1     | 1:A:35:ASP:N        | 2.42                     | 0.50              |
| 27:b:146:LYS:HB2   | 27:b:149:LYS:HB2    | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:i:134:SER:OG    | 51:1:1062:G:N2     | 2.45                     | 0.50              |
| 34:j:2:LYS:HG2     | 51:1:995:C:N4      | 2.27                     | 0.50              |
| 51:1:355:U:H2'     | 51:1:356:G:H8      | 1.77                     | 0.50              |
| 51:1:580:U:O5'     | 51:1:580:U:H6      | 1.94                     | 0.50              |
| 51:1:928:A:O2'     | 51:1:929:U:H5'     | 2.10                     | 0.50              |
| 51:1:1345:C:H6     | 51:1:1345:C:H5'    | 1.77                     | 0.50              |
| 51:1:1409:U:H2'    | 51:1:1410:G:H8     | 1.76                     | 0.50              |
| 51:1:1416:G:H2'    | 51:1:1417:C:C6     | 2.46                     | 0.50              |
| 51:1:1593:A:H2'    | 51:1:1594:U:C6     | 2.47                     | 0.50              |
| 51:1:2734:A:H2'    | 51:1:2735:G:C5'    | 2.42                     | 0.50              |
| 53:3:517:G:N2      | 53:3:533:A:OP2     | 2.33                     | 0.50              |
| 58:B1:412:LEU:HD23 | 58:B1:416:ILE:HG13 | 1.92                     | 0.50              |
| 6:F:19:ARG:HB2     | 6:F:24:ARG:HD2     | 1.92                     | 0.50              |
| 8:H:4:VAL:HG21     | 8:H:9:ILE:HD13     | 1.92                     | 0.50              |
| 15:O:39:PRO:HD2    | 53:3:1123:U:H4'    | 1.92                     | 0.50              |
| 15:O:89:ARG:HH22   | 62:NG:165:PHE:H    | 1.60                     | 0.50              |
| 51:1:1348:C:C5     | 51:1:1349:C:C5     | 3.00                     | 0.50              |
| 51:1:1614:A:H2'    | 51:1:1615:C:H5'    | 1.94                     | 0.50              |
| 51:1:2836:U:H2'    | 51:1:2837:A:C8     | 2.47                     | 0.50              |
| 58:B1:124:ILE:HG23 | 58:B1:128:LEU:HD12 | 1.94                     | 0.50              |
| 58:B1:1371:ARG:HE  | 58:B1:1372:ARG:NH1 | 2.10                     | 0.50              |
| 1:A:37:CYS:O       | 1:A:41:HIS:N       | 2.45                     | 0.50              |
| 12:L:65:LEU:O      | 12:L:69:ARG:N      | 2.43                     | 0.50              |
| 21:U:5:ARG:HB3     | 53:3:376:G:H5''    | 1.93                     | 0.50              |
| 29:d:191:ASP:O     | 29:d:195:GLN:NE2   | 2.44                     | 0.50              |
| 30:e:84:ILE:HD11   | 51:1:2311:A:H1'    | 1.94                     | 0.50              |
| 46:v:51:GLN:OE1    | 46:v:79:ARG:NH2    | 2.40                     | 0.50              |
| 51:1:246:C:H2'     | 51:1:247:G:C5'     | 2.40                     | 0.50              |
| 51:1:900:A:H2'     | 51:1:901:C:H5'     | 1.94                     | 0.50              |
| 51:1:1061:U:H4'    | 51:1:1070:A:H1'    | 1.93                     | 0.50              |
| 51:1:1916:A:H2'    | 51:1:1917:U:O4'    | 2.12                     | 0.50              |
| 51:1:2815:C:O2'    | 51:1:2816:G:H5'    | 2.11                     | 0.50              |
| 59:B2:411:ARG:NH2  | 59:B2:427:ASP:OD2  | 2.44                     | 0.50              |
| 63:5:29:G:H3'      | 63:5:30:G:H8       | 1.76                     | 0.50              |
| 19:S:68:ARG:NH2    | 53:3:974:A:OP1     | 2.45                     | 0.49              |
| 27:b:206:LYS:HD2   | 51:1:729:G:C8      | 2.46                     | 0.49              |
| 43:s:109:ASP:OD1   | 43:s:109:ASP:N     | 2.42                     | 0.49              |
| 51:1:155:A:H2'     | 51:1:156:A:H8      | 1.76                     | 0.49              |
| 51:1:1077:A:H8     | 51:1:1078:U:H1'    | 1.77                     | 0.49              |
| 51:1:1468:U:H2'    | 51:1:1522:A:N6     | 2.26                     | 0.49              |
| 51:1:1528:A:H2'    | 51:1:1529:G:O4'    | 2.11                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:1:1717:A:H2'    | 51:1:1718:G:C5'     | 2.40                     | 0.49              |
| 53:3:928:G:O2'     | 53:3:1533:C:OP1     | 2.22                     | 0.49              |
| 58:B1:421:VAL:O    | 58:B1:436:ALA:HA    | 2.12                     | 0.49              |
| 59:B2:9:LYS:HG2    | 59:B2:1171:ARG:HH12 | 1.77                     | 0.49              |
| 65:0:615:PRO:HG3   | 65:0:687:TYR:HE1    | 1.76                     | 0.49              |
| 7:G:103:TRP:HA     | 7:G:106:VAL:HG12    | 1.93                     | 0.49              |
| 13:M:29:SER:OG     | 13:M:30:LYS:N       | 2.44                     | 0.49              |
| 15:O:42:LEU:HB3    | 15:O:71:LEU:HB2     | 1.94                     | 0.49              |
| 33:i:110:GLN:HG2   | 33:i:121:ILE:HD13   | 1.93                     | 0.49              |
| 33:i:126:ARG:HD2   | 51:1:1080:A:H4'     | 1.93                     | 0.49              |
| 51:1:173:A:H2'     | 51:1:174:U:C6       | 2.47                     | 0.49              |
| 51:1:898:C:H2'     | 51:1:899:A:O4'      | 2.12                     | 0.49              |
| 51:1:1144:A:H2'    | 51:1:1145:C:C6      | 2.47                     | 0.49              |
| 51:1:1645:G:H5''   | 51:1:1646:C:H5'     | 1.94                     | 0.49              |
| 51:1:2298:A:O2'    | 51:1:2299:U:H5'     | 2.12                     | 0.49              |
| 59:B2:232:ILE:HG12 | 59:B2:237:LEU:HG    | 1.94                     | 0.49              |
| 27:b:137:GLY:O     | 27:b:162:GLN:NE2    | 2.45                     | 0.49              |
| 30:e:27:VAL:O      | 30:e:29:ARG:NH1     | 2.41                     | 0.49              |
| 51:1:30:G:H2'      | 51:1:31:C:C6        | 2.47                     | 0.49              |
| 51:1:69:C:O2'      | 51:1:70:G:H5'       | 2.13                     | 0.49              |
| 51:1:236:C:H2'     | 51:1:237:C:C6       | 2.46                     | 0.49              |
| 51:1:1087:G:H2'    | 51:1:1089:A:H5'     | 1.94                     | 0.49              |
| 51:1:2348:U:O2'    | 51:1:2349:G:H5'     | 2.12                     | 0.49              |
| 51:1:2393:U:H2'    | 51:1:2394:C:H5'     | 1.94                     | 0.49              |
| 51:1:2634:A:O2'    | 51:1:2635:A:H5'     | 2.12                     | 0.49              |
| 53:3:481:G:O2'     | 53:3:483:C:N4       | 2.46                     | 0.49              |
| 53:3:1178:G:N2     | 53:3:1181:G:OP2     | 2.43                     | 0.49              |
| 58:B1:1179:PRO:HD2 | 58:B1:1184:ASP:HA   | 1.93                     | 0.49              |
| 7:G:101:THR:HG23   | 7:G:174:GLU:HG3     | 1.95                     | 0.49              |
| 7:G:221:ARG:HG2    | 7:G:224:ARG:HH11    | 1.77                     | 0.49              |
| 16:P:96:ILE:HD13   | 16:P:109:ILE:HD13   | 1.94                     | 0.49              |
| 31:f:41:GLU:HG2    | 31:f:54:ARG:HH21    | 1.78                     | 0.49              |
| 31:f:163:TYR:HB2   | 31:f:166:GLU:HB2    | 1.95                     | 0.49              |
| 44:t:7:LEU:HD13    | 44:t:46:ALA:HA      | 1.94                     | 0.49              |
| 51:1:1119:U:O2'    | 51:1:1120:G:H5'     | 2.13                     | 0.49              |
| 51:1:1785:A:O2'    | 51:1:1786:A:H8      | 1.96                     | 0.49              |
| 31:f:87:GLN:NE2    | 31:f:129:GLU:OE2    | 2.45                     | 0.49              |
| 51:1:16:C:H2'      | 51:1:17:G:H8        | 1.78                     | 0.49              |
| 51:1:519:U:H2'     | 51:1:520:G:C8       | 2.48                     | 0.49              |
| 51:1:644:A:H2'     | 51:1:645:C:C4'      | 2.42                     | 0.49              |
| 51:1:940:G:H2'     | 51:1:941:A:C5'      | 2.41                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:1:1437:C:H2'    | 51:1:1438:U:H6      | 1.78                     | 0.49              |
| 51:1:1539:U:H2'    | 51:1:1540:G:H8      | 1.76                     | 0.49              |
| 51:1:2241:A:O2'    | 51:1:2242:G:H5'     | 2.12                     | 0.49              |
| 51:1:2257:U:O2'    | 51:1:2258:C:H5'     | 2.13                     | 0.49              |
| 51:1:2283:C:H2'    | 51:1:2284:A:O4'     | 2.11                     | 0.49              |
| 51:1:2533:U:H2'    | 51:1:2534:A:C5'     | 2.42                     | 0.49              |
| 27:b:50:THR:HG23   | 51:1:1813:G:N2      | 2.27                     | 0.49              |
| 30:e:57:ALA:HB2    | 30:e:64:PRO:HD3     | 1.95                     | 0.49              |
| 31:f:122:ALA:HB2   | 31:f:132:LEU:HD23   | 1.94                     | 0.49              |
| 51:1:482:A:H1'     | 51:1:498:G:N2       | 2.27                     | 0.49              |
| 51:1:898:C:C2'     | 51:1:899:A:H5'      | 2.43                     | 0.49              |
| 51:1:2281:A:O2'    | 51:1:2282:G:H5'     | 2.12                     | 0.49              |
| 51:1:2290:G:H2'    | 51:1:2291:U:H6      | 1.74                     | 0.49              |
| 51:1:2670:A:O2'    | 51:1:2671:G:H5'     | 2.12                     | 0.49              |
| 17:Q:120:ARG:HH12  | 53:3:500:G:H5'      | 1.77                     | 0.49              |
| 42:r:68:ARG:O      | 42:r:90:ARG:NH2     | 2.46                     | 0.49              |
| 51:1:262:A:H2'     | 51:1:263:G:O4'      | 2.12                     | 0.49              |
| 51:1:367:G:H2'     | 51:1:368:A:O4'      | 2.13                     | 0.49              |
| 51:1:886:A:C5      | 51:1:887:U:H1'      | 2.47                     | 0.49              |
| 51:1:1400:U:H2'    | 51:1:1401:G:H8      | 1.78                     | 0.49              |
| 57:A1:18:GLN:HA    | 57:A1:24:ALA:HA     | 1.94                     | 0.49              |
| 58:B1:220:ARG:HG2  | 58:B1:220:ARG:NH1   | 2.25                     | 0.49              |
| 7:G:18:GLN:HG3     | 7:G:189:ASN:CB      | 2.41                     | 0.49              |
| 12:L:2:ARG:NH2     | 53:3:933:G:O6       | 2.45                     | 0.49              |
| 14:N:94:ARG:HG2    | 14:N:97:LEU:HD12    | 1.95                     | 0.49              |
| 29:d:77:ILE:HG23   | 51:1:1256:G:N2      | 2.26                     | 0.49              |
| 48:x:1:SER:O       | 48:x:49:ARG:NH1     | 2.46                     | 0.49              |
| 51:1:131:A:H2'     | 51:1:132:G:H8       | 1.77                     | 0.49              |
| 51:1:840:C:O2'     | 51:1:841:G:H5'      | 2.12                     | 0.49              |
| 58:B1:115:TRP:O    | 58:B1:1333:THR:HG21 | 2.13                     | 0.49              |
| 59:B2:529:ARG:HH11 | 59:B2:572:ILE:HG22  | 1.77                     | 0.49              |
| 9:I:153:ARG:NH2    | 53:3:435:A:N3       | 2.61                     | 0.49              |
| 21:U:36:VAL:HG12   | 21:U:53:ASP:HB3     | 1.94                     | 0.49              |
| 28:c:81:GLU:HG3    | 51:1:2636:C:O5'     | 2.13                     | 0.49              |
| 33:i:20:SER:H      | 33:i:21:PRO:HD2     | 1.78                     | 0.49              |
| 33:i:79:LEU:HD13   | 33:i:132:ALA:HB2    | 1.94                     | 0.49              |
| 41:q:103:VAL:HA    | 41:q:106:THR:HG22   | 1.94                     | 0.49              |
| 44:t:70:HIS:N      | 44:t:73:ARG:O       | 2.44                     | 0.49              |
| 51:1:609:A:H2'     | 51:1:610:C:O4'      | 2.11                     | 0.49              |
| 51:1:841:G:C2      | 51:1:938:G:C2       | 3.01                     | 0.49              |
| 51:1:1117:C:H2'    | 51:1:1118:C:H6      | 1.78                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:1:1668:A:N3     | 51:1:1670:C:N4      | 2.60                     | 0.49              |
| 51:1:1910:G:N2     | 51:1:1911:U:C2      | 2.81                     | 0.49              |
| 53:3:1137:C:H4'    | 53:3:1138:G:H5'     | 1.94                     | 0.49              |
| 58:B1:145:VAL:HG12 | 58:B1:184:ALA:HB1   | 1.94                     | 0.49              |
| 58:B1:902:ASP:HB3  | 58:B1:905:ARG:HB2   | 1.93                     | 0.49              |
| 59:B2:554:HIS:HD2  | 59:B2:558:VAL:HB    | 1.77                     | 0.49              |
| 65:0:616:ILE:HB    | 65:0:686:LYS:HE3    | 1.95                     | 0.49              |
| 14:N:91:GLU:HA     | 14:N:94:ARG:HB2     | 1.94                     | 0.49              |
| 28:c:56:LYS:NZ     | 51:1:2830:C:H5''    | 2.28                     | 0.49              |
| 33:i:85:ILE:HD12   | 33:i:97:VAL:HG12    | 1.95                     | 0.49              |
| 37:m:74:THR:HG21   | 37:m:86:LYS:HG2     | 1.94                     | 0.49              |
| 51:1:67:U:H2'      | 51:1:68:G:H8        | 1.77                     | 0.49              |
| 51:1:1534:U:H4'    | 51:1:1535:A:N1      | 2.27                     | 0.49              |
| 51:1:1796:U:H2'    | 51:1:1797:G:C8      | 2.45                     | 0.49              |
| 51:1:2843:G:O2'    | 51:1:2844:G:H5'     | 2.13                     | 0.49              |
| 38:n:8:ARG:HH21    | 38:n:43:GLU:HG3     | 1.77                     | 0.48              |
| 51:1:118:A:H2'     | 51:1:120:U:O4       | 2.13                     | 0.48              |
| 51:1:898:C:O2'     | 51:1:899:A:H5'      | 2.13                     | 0.48              |
| 51:1:1111:A:H2'    | 51:1:1111:A:N3      | 2.28                     | 0.48              |
| 51:1:1537:G:H3'    | 51:1:1537:G:N3      | 2.28                     | 0.48              |
| 51:1:2050:C:N4     | 51:1:2051:A:C6      | 2.81                     | 0.48              |
| 51:1:2126:A:H5'    | 51:1:2127:G:O5'     | 2.13                     | 0.48              |
| 51:1:2510:C:N4     | 51:1:2511:U:C4      | 2.81                     | 0.48              |
| 53:3:890:G:O2'     | 53:3:906:A:N6       | 2.46                     | 0.48              |
| 53:3:1064:G:O2'    | 53:3:1190:G:N2      | 2.46                     | 0.48              |
| 59:B2:836:LEU:HD13 | 59:B2:1054:LEU:HD13 | 1.95                     | 0.48              |
| 9:I:93:LEU:O       | 9:I:99:ASN:ND2      | 2.39                     | 0.48              |
| 25:Y:59:ARG:O      | 25:Y:63:LYS:N       | 2.46                     | 0.48              |
| 51:1:78:U:H2'      | 51:1:79:C:H6        | 1.77                     | 0.48              |
| 51:1:121:G:H4'     | 51:1:149:A:H5'      | 1.95                     | 0.48              |
| 51:1:129:C:H2'     | 51:1:130:C:H6       | 1.79                     | 0.48              |
| 51:1:1084:A:O2'    | 51:1:1105:U:H4'     | 2.12                     | 0.48              |
| 51:1:1536:C:H5''   | 51:1:1537:G:C4      | 2.48                     | 0.48              |
| 51:1:2208:C:H2'    | 51:1:2209:G:C8      | 2.48                     | 0.48              |
| 55:8:3:DC:H2''     | 55:8:4:DT:C7        | 2.42                     | 0.48              |
| 17:Q:97:VAL:HG12   | 17:Q:99:GLY:H       | 1.78                     | 0.48              |
| 27:b:70:LYS:O      | 27:b:117:SER:OG     | 2.30                     | 0.48              |
| 51:1:54:G:H2'      | 51:1:55:G:O4'       | 2.12                     | 0.48              |
| 51:1:360:U:H2'     | 51:1:361:G:C1'      | 2.43                     | 0.48              |
| 51:1:473:G:O2'     | 51:1:474:G:H5'      | 2.14                     | 0.48              |
| 51:1:572:A:H8      | 51:1:572:A:O5'      | 1.97                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1:706:A:H2'     | 51:1:707:G:H5'     | 1.95                     | 0.48              |
| 51:1:1680:U:O2'    | 51:1:1681:G:H5'    | 2.13                     | 0.48              |
| 51:1:2180:U:O2'    | 51:1:2181:U:H5'    | 2.13                     | 0.48              |
| 51:1:2367:G:O2'    | 51:1:2368:C:H5'    | 2.13                     | 0.48              |
| 52:2:51:G:H22      | 52:2:53:A:H62      | 1.61                     | 0.48              |
| 58:B1:1027:VAL:HB  | 58:B1:1121:LEU:HB2 | 1.95                     | 0.48              |
| 9:I:94:GLU:HG3     | 9:I:190:LEU:HD21   | 1.95                     | 0.48              |
| 17:Q:110:LYS:HG3   | 17:Q:121:PRO:HG3   | 1.94                     | 0.48              |
| 25:Y:53:MET:HE2    | 25:Y:57:VAL:HG21   | 1.94                     | 0.48              |
| 35:k:5:GLN:HE21    | 51:1:1668:A:H5''   | 1.78                     | 0.48              |
| 51:1:214:G:H2'     | 51:1:215:G:C8      | 2.48                     | 0.48              |
| 51:1:286:U:H2'     | 51:1:287:G:C8      | 2.47                     | 0.48              |
| 51:1:1742:U:O2'    | 51:1:1743:G:H5'    | 2.14                     | 0.48              |
| 51:1:1748:C:H2'    | 51:1:1749:A:C8     | 2.47                     | 0.48              |
| 51:1:2214:C:H2'    | 51:1:2215:C:O4'    | 2.14                     | 0.48              |
| 51:1:2329:U:H2'    | 51:1:2330:G:H8     | 1.78                     | 0.48              |
| 53:3:673:A:H2'     | 53:3:674:G:C8      | 2.49                     | 0.48              |
| 58:B1:809:VAL:HG21 | 58:B1:909:ILE:HG12 | 1.95                     | 0.48              |
| 58:B1:968:ASN:HA   | 58:B1:1117:SER:HB2 | 1.96                     | 0.48              |
| 59:B2:18:ARG:HE    | 59:B2:620:ASN:HA   | 1.77                     | 0.48              |
| 59:B2:533:LEU:HD13 | 59:B2:540:ARG:HH21 | 1.77                     | 0.48              |
| 12:L:41:ILE:HD11   | 53:3:1240:U:H5'    | 1.94                     | 0.48              |
| 29:d:143:LEU:HD13  | 29:d:146:VAL:HG11  | 1.94                     | 0.48              |
| 45:u:88:ASP:OD1    | 45:u:88:ASP:N      | 2.43                     | 0.48              |
| 51:1:217:A:H2'     | 51:1:218:A:O4'     | 2.13                     | 0.48              |
| 51:1:488:G:H22     | 51:1:491:G:H5''    | 1.77                     | 0.48              |
| 51:1:553:G:H2'     | 51:1:554:U:O4'     | 2.13                     | 0.48              |
| 51:1:1087:G:O6     | 51:1:1089:A:C2     | 2.67                     | 0.48              |
| 51:1:2649:C:O2'    | 51:1:2650:U:H5'    | 2.13                     | 0.48              |
| 53:3:1531:A:O2'    | 53:3:1532:U:H5'    | 2.14                     | 0.48              |
| 57:A1:100:LEU:HB2  | 57:A1:144:ILE:HG23 | 1.94                     | 0.48              |
| 59:B2:857:VAL:HG13 | 59:B2:919:ARG:HH21 | 1.78                     | 0.48              |
| 63:5:51:U:H2'      | 63:5:52:G:C8       | 2.48                     | 0.48              |
| 6:F:6:SER:O        | 6:F:6:SER:OG       | 2.31                     | 0.48              |
| 42:r:71:LYS:HA     | 42:r:90:ARG:HG2    | 1.95                     | 0.48              |
| 51:1:92:U:H2'      | 51:1:93:G:H5'      | 1.96                     | 0.48              |
| 51:1:481:G:C2'     | 51:1:482:A:OP2     | 2.61                     | 0.48              |
| 51:1:1871:A:H2'    | 51:1:1872:A:O4'    | 2.13                     | 0.48              |
| 53:3:880:C:H2'     | 53:3:881:G:H8      | 1.78                     | 0.48              |
| 14:N:10:ARG:NH2    | 53:3:1119:C:OP2    | 2.46                     | 0.48              |
| 17:Q:82:ARG:O      | 17:Q:95:HIS:N      | 2.47                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 26:Z:55:HIS:HA     | 26:Z:58:LYS:HD2     | 1.95                     | 0.48              |
| 51:1:718:A:H2'     | 51:1:719:C:O4'      | 2.12                     | 0.48              |
| 51:1:2016:U:O5'    | 51:1:2016:U:H6      | 1.97                     | 0.48              |
| 51:1:2828:G:O2'    | 51:1:2829:A:H5'     | 2.13                     | 0.48              |
| 58:B1:102:MET:HG2  | 58:B1:246:PRO:HD3   | 1.94                     | 0.48              |
| 58:B1:201:LEU:HD11 | 58:B1:220:ARG:HG2   | 1.95                     | 0.48              |
| 58:B1:352:ARG:HD2  | 59:B2:1268:GLN:HE21 | 1.68                     | 0.48              |
| 64:6:50:U:H2'      | 64:6:51:C:C5        | 2.49                     | 0.48              |
| 32:g:8:LYS:HD3     | 32:g:14:SER:HA      | 1.96                     | 0.48              |
| 38:n:100:CYS:H     | 38:n:111:ALA:HA     | 1.79                     | 0.48              |
| 49:y:16:THR:O      | 49:y:20:ASN:ND2     | 2.46                     | 0.48              |
| 51:1:415:A:H2'     | 51:1:416:U:C6       | 2.49                     | 0.48              |
| 51:1:596:U:C2      | 51:1:662:G:N2       | 2.82                     | 0.48              |
| 51:1:852:U:H2'     | 51:1:853:C:C6       | 2.49                     | 0.48              |
| 51:1:1807:G:C2'    | 51:1:1808:A:H5'     | 2.29                     | 0.48              |
| 51:1:2547:A:H61    | 51:1:2561:U:H3      | 1.62                     | 0.48              |
| 53:3:38:G:H22      | 53:3:397:A:H5'      | 1.78                     | 0.48              |
| 55:8:14:DC:H2'     | 55:8:15:DC:C6       | 2.48                     | 0.48              |
| 58:B1:190:LYS:HB2  | 58:B1:190:LYS:HE3   | 1.41                     | 0.48              |
| 58:B1:1036:ARG:HE  | 58:B1:1081:VAL:HG11 | 1.79                     | 0.48              |
| 59:B2:400:VAL:HG22 | 59:B2:584:TYR:HB3   | 1.96                     | 0.48              |
| 62:NG:161:SER:CA   | 62:NG:170:PRO:HA    | 2.43                     | 0.48              |
| 14:N:44:ARG:O      | 14:N:47:VAL:HG22    | 2.13                     | 0.48              |
| 14:N:86:LEU:HD12   | 14:N:97:LEU:HD11    | 1.95                     | 0.48              |
| 36:l:129:LYS:HG2   | 51:1:636:G:OP1      | 2.14                     | 0.48              |
| 39:o:15:ARG:NH2    | 52:2:8:C:OP1        | 2.47                     | 0.48              |
| 51:1:555:G:O2'     | 51:1:556:A:H8       | 1.96                     | 0.48              |
| 51:1:1464:G:H2'    | 51:1:1465:G:C8      | 2.49                     | 0.48              |
| 51:1:1465:G:H2'    | 51:1:1466:U:O4'     | 2.13                     | 0.48              |
| 51:1:2527:C:O2'    | 51:1:2528:U:H5'     | 2.13                     | 0.48              |
| 53:3:401:C:O2'     | 53:3:621:A:N3       | 2.45                     | 0.48              |
| 53:3:776:G:N2      | 53:3:802:A:OP2      | 2.39                     | 0.48              |
| 58:B1:255:LEU:HD23 | 58:B1:261:ALA:HB2   | 1.95                     | 0.48              |
| 58:B1:891:ASP:OD2  | 58:B1:1290:ARG:NH2  | 2.47                     | 0.48              |
| 59:B2:732:ILE:HD11 | 59:B2:769:PRO:HB3   | 1.95                     | 0.48              |
| 59:B2:895:LEU:HD12 | 59:B2:899:GLU:HB3   | 1.95                     | 0.48              |
| 29:d:149:ILE:HD11  | 29:d:172:ALA:HA     | 1.96                     | 0.48              |
| 31:f:16:VAL:HA     | 31:f:25:ILE:HG12    | 1.96                     | 0.48              |
| 51:1:275:C:C3'     | 51:1:276:U:H5''     | 2.40                     | 0.48              |
| 51:1:476:G:H4'     | 51:1:502:A:N1       | 2.28                     | 0.48              |
| 51:1:820:A:H2'     | 51:1:821:A:O4'      | 2.14                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 51:1:854:C:H2'      | 51:1:855:G:H8       | 1.79                     | 0.48              |
| 51:1:1387:A:C5'     | 51:1:1469:A:H1'     | 2.38                     | 0.48              |
| 51:1:2660:A:N6      | 65:0:672:SER:HB2    | 2.29                     | 0.48              |
| 53:3:898:G:N2       | 53:3:901:A:OP2      | 2.46                     | 0.48              |
| 58:B1:108:ALA:HB1   | 58:B1:279:LEU:HD22  | 1.96                     | 0.48              |
| 63:5:50:U:H2'       | 63:5:51:U:C6        | 2.49                     | 0.48              |
| 27:b:152:GLN:HB3    | 51:1:1818:U:N3      | 2.29                     | 0.47              |
| 29:d:48:THR:OG1     | 29:d:49:ARG:N       | 2.47                     | 0.47              |
| 29:d:119:ILE:HB     | 29:d:187:VAL:HG12   | 1.96                     | 0.47              |
| 40:p:2:ASN:HD21     | 51:1:2876:G:H4'     | 1.79                     | 0.47              |
| 51:1:2098:U:H2'     | 51:1:2099:U:O4'     | 2.14                     | 0.47              |
| 51:1:2149:U:H2'     | 51:1:2150:C:C6      | 2.49                     | 0.47              |
| 51:1:2286:G:H21     | 51:1:2287:A:H61     | 1.62                     | 0.47              |
| 53:3:1305:G:N2      | 53:3:1331:G:H2'     | 2.29                     | 0.47              |
| 58:B1:103:GLY:H     | 58:B1:244:VAL:HG22  | 1.79                     | 0.47              |
| 58:B1:550:VAL:O     | 58:B1:569:LEU:HA    | 2.13                     | 0.47              |
| 58:B1:1146:GLU:OE2  | 58:B1:1310:THR:HG22 | 2.14                     | 0.47              |
| 12:L:112:ASP:HB2    | 12:L:118:ARG:HG2    | 1.97                     | 0.47              |
| 17:Q:70:GLY:O       | 17:Q:98:ARG:NH2     | 2.47                     | 0.47              |
| 28:c:190:LYS:HE2    | 51:1:2729:G:H4'     | 1.95                     | 0.47              |
| 32:g:47:PHE:HA      | 32:g:51:ARG:HB2     | 1.96                     | 0.47              |
| 33:i:54:ILE:HD12    | 33:i:73:PRO:HD3     | 1.95                     | 0.47              |
| 40:p:59:THR:HG22    | 40:p:72:VAL:HG12    | 1.95                     | 0.47              |
| 42:r:7:SER:OG       | 42:r:8:GLY:N        | 2.47                     | 0.47              |
| 47:w:29:ALA:N       | 47:w:60:ASP:OD1     | 2.48                     | 0.47              |
| 51:1:5:A:H2'        | 51:1:6:A:C8         | 2.49                     | 0.47              |
| 51:1:40:U:H2'       | 51:1:41:C:H6        | 1.78                     | 0.47              |
| 51:1:813:U:C2       | 51:1:1195:G:N2      | 2.83                     | 0.47              |
| 51:1:1026:G:OP2     | 51:1:1134:A:H1'     | 2.13                     | 0.47              |
| 51:1:2362:C:O5'     | 51:1:2362:C:H6      | 1.96                     | 0.47              |
| 53:3:1223:C:H5'     | 53:3:1224:U:H5''    | 1.96                     | 0.47              |
| 58:B1:1060:VAL:HG13 | 58:B1:1106:ILE:HG12 | 1.96                     | 0.47              |
| 20:T:38:LEU:HD22    | 20:T:55:LEU:HD13    | 1.96                     | 0.47              |
| 21:U:18:GLN:HA      | 21:U:38:PHE:HA      | 1.95                     | 0.47              |
| 27:b:131:MET:HE2    | 27:b:187:CYS:HB2    | 1.96                     | 0.47              |
| 51:1:107:G:O2'      | 51:1:108:G:H5'      | 2.14                     | 0.47              |
| 51:1:554:U:O2'      | 51:1:555:G:H5'      | 2.13                     | 0.47              |
| 51:1:762:U:N3       | 51:1:1431:A:OP1     | 2.47                     | 0.47              |
| 51:1:1463:C:H2'     | 51:1:1464:G:C8      | 2.49                     | 0.47              |
| 51:1:2156:G:C3'     | 51:1:2157:G:H5'     | 2.44                     | 0.47              |
| 51:1:2899:A:H2'     | 51:1:2900:A:O4'     | 2.15                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 53:3:816:A:OP1      | 53:3:1526:G:O2'     | 2.28                     | 0.47              |
| 58:B1:375:GLU:HB3   | 59:B2:1245:ALA:HB3  | 1.97                     | 0.47              |
| 58:B1:1347:LEU:HG   | 58:B1:1357:ILE:HG23 | 1.96                     | 0.47              |
| 59:B2:1311:GLY:O    | 60:W0:31:GLN:NE2    | 2.47                     | 0.47              |
| 59:B2:1314:GLN:HB2  | 60:W0:28:ARG:HH12   | 1.79                     | 0.47              |
| 65:0:12:ASN:HB2     | 65:0:107:ASP:OD2    | 2.14                     | 0.47              |
| 27:b:156:SER:OG     | 27:b:157:ALA:N      | 2.44                     | 0.47              |
| 31:f:133:LYS:NZ     | 31:f:134:GLY:O      | 2.44                     | 0.47              |
| 31:f:174:LYS:HD2    | 31:f:176:LYS:HB2    | 1.96                     | 0.47              |
| 45:u:39:ASN:HB3     | 45:u:62:ALA:HB3     | 1.95                     | 0.47              |
| 51:1:143:C:H2'      | 51:1:144:A:C8       | 2.49                     | 0.47              |
| 51:1:1019:U:N3      | 51:1:1142:A:N6      | 2.57                     | 0.47              |
| 51:1:1067:A:H2'     | 51:1:1068:G:C8      | 2.49                     | 0.47              |
| 51:1:2298:A:C2'     | 51:1:2299:U:H5'     | 2.45                     | 0.47              |
| 51:1:2626:C:H2'     | 51:1:2627:G:H8      | 1.80                     | 0.47              |
| 51:1:2895:G:H2'     | 51:1:2896:C:C6      | 2.49                     | 0.47              |
| 53:3:768:A:N3       | 53:3:1512:U:O2'     | 2.46                     | 0.47              |
| 58:B1:395:LYS:NZ    | 58:B1:399:LYS:CE    | 2.77                     | 0.47              |
| 58:B1:1221:LEU:HD22 | 58:B1:1306:LEU:HB2  | 1.96                     | 0.47              |
| 59:B2:565:GLU:HA    | 59:B2:569:ILE:HG12  | 1.95                     | 0.47              |
| 18:R:15:VAL:HG11    | 18:R:30:LYS:HG2     | 1.97                     | 0.47              |
| 28:c:13:ARG:NH2     | 40:p:74:GLN:OE1     | 2.43                     | 0.47              |
| 47:w:19:VAL:HA      | 47:w:34:VAL:HG22    | 1.97                     | 0.47              |
| 51:1:712:G:H2'      | 51:1:713:G:H5'      | 1.96                     | 0.47              |
| 51:1:1257:C:O5'     | 51:1:1257:C:H6      | 1.97                     | 0.47              |
| 51:1:1464:G:H2'     | 51:1:1465:G:H8      | 1.78                     | 0.47              |
| 51:1:1922:G:H2'     | 51:1:1923:U:C6      | 2.50                     | 0.47              |
| 51:1:2455:G:C6      | 51:1:2456:C:N4      | 2.83                     | 0.47              |
| 53:3:358:U:H2'      | 53:3:359:G:H8       | 1.78                     | 0.47              |
| 57:A1:182:ARG:O     | 57:A1:205:MET:HA    | 2.14                     | 0.47              |
| 58:B1:1357:ILE:HD13 | 59:B2:1279:GLU:HG2  | 1.97                     | 0.47              |
| 59:B2:207:THR:OG1   | 59:B2:354:ASP:OD2   | 2.32                     | 0.47              |
| 5:E:5:THR:HG22      | 5:E:62:PRO:HD2      | 1.97                     | 0.47              |
| 15:O:58:ASN:ND2     | 53:3:1061:G:O2'     | 2.45                     | 0.47              |
| 31:f:88:LEU:HD21    | 31:f:104:LEU:HD23   | 1.97                     | 0.47              |
| 51:1:551:G:O2'      | 51:1:552:U:H5'      | 2.15                     | 0.47              |
| 51:1:1098:A:O2'     | 51:1:1099:G:H5'     | 2.15                     | 0.47              |
| 57:A1:59:VAL:HG22   | 57:A1:144:ILE:HA    | 1.97                     | 0.47              |
| 58:B1:1261:LEU:HD12 | 58:B1:1304:ARG:HH21 | 1.78                     | 0.47              |
| 59:B2:103:VAL:HG12  | 59:B2:117:ILE:HG22  | 1.97                     | 0.47              |
| 4:D:29:GLN:O        | 4:D:29:GLN:NE2      | 2.47                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:I:159:GLU:HA     | 9:I:162:GLU:HB2   | 1.97                     | 0.47              |
| 12:L:107:ALA:HA    | 12:L:122:GLU:HG3  | 1.95                     | 0.47              |
| 12:L:149:ALA:HB1   | 16:P:58:THR:HG21  | 1.97                     | 0.47              |
| 21:U:25:ARG:NH1    | 53:3:230:G:O2'    | 2.48                     | 0.47              |
| 28:c:136:ASN:OD1   | 51:1:2579:C:O2'   | 2.32                     | 0.47              |
| 46:v:79:ARG:HA     | 46:v:86:LEU:HA    | 1.95                     | 0.47              |
| 51:1:283:G:C2'     | 51:1:284:U:H5'    | 2.45                     | 0.47              |
| 51:1:368:A:H2'     | 51:1:369:U:C5'    | 2.39                     | 0.47              |
| 51:1:1020:A:C1'    | 51:1:1021:A:OP2   | 2.61                     | 0.47              |
| 51:1:1367:A:H3'    | 51:1:1368:G:O4'   | 2.15                     | 0.47              |
| 51:1:1435:G:O2'    | 51:1:1436:G:H5'   | 2.15                     | 0.47              |
| 51:1:1702:G:H2'    | 51:1:1703:G:C5'   | 2.35                     | 0.47              |
| 51:1:1726:C:H2'    | 51:1:1727:C:C6    | 2.50                     | 0.47              |
| 51:1:1729:U:H5     | 51:1:1731:G:N2    | 2.12                     | 0.47              |
| 51:1:2155:U:H2'    | 51:1:2156:G:O4'   | 2.15                     | 0.47              |
| 51:1:2194:U:O2'    | 51:1:2195:U:H5'   | 2.14                     | 0.47              |
| 51:1:2395:C:H2'    | 51:1:2396:G:O4'   | 2.15                     | 0.47              |
| 51:1:2445:G:C6     | 51:1:2446:G:C6    | 3.02                     | 0.47              |
| 51:1:2554:U:H2'    | 51:1:2555:U:O2    | 2.15                     | 0.47              |
| 51:1:2625:G:H2'    | 51:1:2626:C:H6    | 1.76                     | 0.47              |
| 53:3:944:G:N1      | 53:3:1338:G:OP2   | 2.34                     | 0.47              |
| 58:B1:43:THR:HG22  | 58:B1:57:PHE:HE1  | 1.80                     | 0.47              |
| 58:B1:526:VAL:HG12 | 58:B1:549:LYS:HB2 | 1.96                     | 0.47              |
| 16:P:34:THR:OG1    | 16:P:35:ASP:N     | 2.47                     | 0.47              |
| 19:S:32:ASP:O      | 19:S:34:ASN:ND2   | 2.48                     | 0.47              |
| 43:s:72:THR:OG1    | 43:s:73:LYS:N     | 2.48                     | 0.47              |
| 45:u:6:ARG:HB2     | 51:1:85:G:P       | 2.55                     | 0.47              |
| 51:1:297:G:H2'     | 51:1:298:G:O4'    | 2.14                     | 0.47              |
| 51:1:877:A:O2'     | 51:1:878:A:H5''   | 2.14                     | 0.47              |
| 51:1:1219:U:O2'    | 51:1:1220:G:H5'   | 2.15                     | 0.47              |
| 51:1:1517:G:O2'    | 51:1:1518:C:H5'   | 2.15                     | 0.47              |
| 51:1:2563:U:H2'    | 51:1:2565:A:OP2   | 2.15                     | 0.47              |
| 58:B1:141:PHE:HE2  | 58:B1:296:LYS:CB  | 2.22                     | 0.47              |
| 58:B1:1361:THR:OG1 | 59:B2:1282:GLY:O  | 2.28                     | 0.47              |
| 63:5:8:U:H2'       | 63:5:13:C:N4      | 2.30                     | 0.47              |
| 51:1:149:A:H2'     | 51:1:150:U:C6     | 2.49                     | 0.47              |
| 51:1:466:A:H2'     | 51:1:467:G:C5'    | 2.44                     | 0.47              |
| 51:1:900:A:C2'     | 51:1:901:C:H5'    | 2.45                     | 0.47              |
| 51:1:979:A:H2'     | 51:1:982:C:H42    | 1.80                     | 0.47              |
| 51:1:1068:G:H2'    | 51:1:1069:A:H4'   | 1.96                     | 0.47              |
| 51:1:1297:C:H2'    | 51:1:1298:C:H6    | 1.79                     | 0.47              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 51:1:1400:U:H2'   | 51:1:1401:G:C8      | 2.50                     | 0.47              |
| 51:1:1491:G:H2'   | 51:1:1492:G:H8      | 1.80                     | 0.47              |
| 51:1:1873:G:O2'   | 51:1:1874:C:H5'     | 2.15                     | 0.47              |
| 51:1:1922:G:O2'   | 51:1:1923:U:H5'     | 2.15                     | 0.47              |
| 51:1:2180:U:H2'   | 51:1:2181:U:O4'     | 2.14                     | 0.47              |
| 51:1:2259:U:H2'   | 51:1:2260:C:O4'     | 2.15                     | 0.47              |
| 51:1:2581:G:H2'   | 51:1:2581:G:N3      | 2.30                     | 0.47              |
| 53:3:617:G:H1     | 53:3:623:C:H42      | 1.63                     | 0.47              |
| 57:A2:64:VAL:HG11 | 57:A2:78:ILE:HG21   | 1.97                     | 0.47              |
| 58:B1:352:ARG:HB2 | 59:B2:1268:GLN:NE2  | 2.30                     | 0.47              |
| 58:B1:420:PRO:HA  | 58:B1:437:PHE:O     | 2.15                     | 0.47              |
| 59:B2:689:ALA:HB2 | 59:B2:1233:LEU:HD23 | 1.97                     | 0.47              |
| 64:6:48:C:H5''    | 64:6:50:U:OP1       | 2.15                     | 0.47              |
| 9:I:171:GLU:HB3   | 9:I:180:THR:HG22    | 1.97                     | 0.47              |
| 12:L:79:VAL:HB    | 12:L:84:TYR:HD2     | 1.80                     | 0.47              |
| 31:f:100:ASN:OD1  | 31:f:100:ASN:N      | 2.47                     | 0.47              |
| 33:i:115:ASP:OD2  | 51:1:1059:G:H4'     | 2.14                     | 0.47              |
| 46:v:83:LYS:HB3   | 46:v:85:LYS:HZ3     | 1.79                     | 0.47              |
| 51:1:435:C:C2'    | 51:1:436:C:H5'      | 2.44                     | 0.47              |
| 51:1:686:U:H6     | 51:1:788:A:H61      | 1.61                     | 0.47              |
| 51:1:708:G:H2'    | 51:1:709:U:C6       | 2.50                     | 0.47              |
| 51:1:859:G:C2'    | 51:1:860:U:OP2      | 2.62                     | 0.47              |
| 51:1:1209:U:O3'   | 51:1:1212:G:H5'     | 2.15                     | 0.47              |
| 51:1:1267:U:H2'   | 51:1:1267:U:O2      | 2.14                     | 0.47              |
| 51:1:1913:A:C8    | 53:3:1494:G:H4'     | 2.50                     | 0.47              |
| 51:1:2295:C:O2'   | 51:1:2296:U:H5'     | 2.15                     | 0.47              |
| 51:1:2858:C:H2'   | 51:1:2859:G:O4'     | 2.15                     | 0.47              |
| 7:G:129:THR:HB    | 7:G:132:GLU:HB2     | 1.96                     | 0.46              |
| 18:R:7:ASN:HD22   | 18:R:20:SER:HB2     | 1.80                     | 0.46              |
| 20:T:37:HIS:HD2   | 20:T:38:LEU:HD12    | 1.80                     | 0.46              |
| 27:b:184:GLU:HG3  | 27:b:186:ASP:H      | 1.80                     | 0.46              |
| 39:o:68:LYS:HE3   | 52:2:49:C:H5''      | 1.97                     | 0.46              |
| 51:1:214:G:O2'    | 51:1:215:G:H5'      | 2.14                     | 0.46              |
| 51:1:570:G:H5'    | 51:1:983:A:C2       | 2.51                     | 0.46              |
| 51:1:1036:G:O2'   | 51:1:1037:G:H5'     | 2.15                     | 0.46              |
| 51:1:1465:G:HO2'  | 51:1:1466:U:H5'     | 1.80                     | 0.46              |
| 51:1:1480:C:H2'   | 51:1:1481:U:C6      | 2.49                     | 0.46              |
| 51:1:1536:C:H5''  | 51:1:1537:G:C5      | 2.50                     | 0.46              |
| 51:1:2047:C:O5'   | 51:1:2047:C:H6      | 1.98                     | 0.46              |
| 51:1:2241:A:H2'   | 51:1:2242:G:C8      | 2.50                     | 0.46              |
| 51:1:2360:G:H2'   | 51:1:2361:G:C5'     | 2.40                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 53:3:410:G:H21     | 53:3:432:A:H62      | 1.62                     | 0.46              |
| 53:3:1225:A:H2'    | 53:3:1225:A:N3      | 2.29                     | 0.46              |
| 58:B1:833:GLU:N    | 58:B1:1242:ARG:HH12 | 2.12                     | 0.46              |
| 58:B1:1150:PRO:HG3 | 58:B1:1214:PRO:HB2  | 1.97                     | 0.46              |
| 48:x:14:GLY:HA3    | 48:x:28:PHE:HE1     | 1.81                     | 0.46              |
| 51:1:156:A:H2'     | 51:1:157:C:C6       | 2.50                     | 0.46              |
| 51:1:389:G:O2'     | 51:1:390:U:H5'      | 2.15                     | 0.46              |
| 51:1:1141:U:H4'    | 51:1:1142:A:C1'     | 2.45                     | 0.46              |
| 51:1:1146:C:O2'    | 51:1:1147:A:H5'     | 2.16                     | 0.46              |
| 51:1:1389:G:C2     | 51:1:1390:U:C2      | 3.02                     | 0.46              |
| 51:1:1516:G:O2'    | 51:1:1517:G:H5'     | 2.15                     | 0.46              |
| 51:1:1528:A:H2'    | 51:1:1529:G:C5'     | 2.44                     | 0.46              |
| 51:1:1851:U:OP1    | 64:6:4:G:H4'        | 2.15                     | 0.46              |
| 51:1:2496:C:H2'    | 51:1:2497:A:O4'     | 2.16                     | 0.46              |
| 53:3:459:A:H2'     | 53:3:460:A:C8       | 2.50                     | 0.46              |
| 59:B2:28:LEU:HD21  | 59:B2:524:ILE:HG13  | 1.98                     | 0.46              |
| 65:0:93:VAL:HA     | 65:0:96:THR:HG23    | 1.97                     | 0.46              |
| 65:0:97:ILE:HD11   | 65:0:411:PHE:HD1    | 1.80                     | 0.46              |
| 35:k:47:ILE:HG22   | 35:k:49:ARG:H       | 1.80                     | 0.46              |
| 36:l:39:LYS:HG2    | 51:1:832:U:OP1      | 2.15                     | 0.46              |
| 46:v:26:PHE:HE2    | 46:v:89:ILE:HG13    | 1.80                     | 0.46              |
| 51:1:93:G:O2'      | 51:1:94:A:H5'       | 2.16                     | 0.46              |
| 51:1:536:G:H2'     | 51:1:537:G:C5'      | 2.43                     | 0.46              |
| 51:1:1874:C:H2'    | 51:1:1875:G:O4'     | 2.15                     | 0.46              |
| 51:1:2290:G:O2'    | 51:1:2291:U:H5'     | 2.16                     | 0.46              |
| 51:1:2350:C:H2'    | 51:1:2351:G:O4'     | 2.16                     | 0.46              |
| 53:3:512:U:H2'     | 53:3:513:C:C6       | 2.50                     | 0.46              |
| 53:3:959:A:O2'     | 53:3:984:C:O2'      | 2.24                     | 0.46              |
| 53:3:1035:A:H1'    | 53:3:1036:A:O5'     | 2.16                     | 0.46              |
| 58:B1:29:MET:HG2   | 59:B2:1336:ASN:ND2  | 2.29                     | 0.46              |
| 59:B2:363:LEU:HB3  | 59:B2:381:ALA:HB1   | 1.96                     | 0.46              |
| 59:B2:562:GLU:OE1  | 59:B2:662:SER:OG    | 2.28                     | 0.46              |
| 10:J:73:VAL:HG11   | 10:J:143:LEU:HB3    | 1.98                     | 0.46              |
| 27:b:145:MET:HE1   | 51:1:1800:C:H2'     | 1.98                     | 0.46              |
| 31:f:29:ASN:ND2    | 31:f:80:GLU:O       | 2.48                     | 0.46              |
| 34:j:65:THR:HG22   | 51:1:1141:U:OP2     | 2.15                     | 0.46              |
| 49:y:15:ASN:OD1    | 49:y:16:THR:N       | 2.48                     | 0.46              |
| 51:1:30:G:C5       | 51:1:31:C:C4        | 3.03                     | 0.46              |
| 51:1:289:G:H2'     | 51:1:290:U:C6       | 2.50                     | 0.46              |
| 51:1:554:U:C2'     | 51:1:555:G:H5'      | 2.46                     | 0.46              |
| 51:1:595:C:C2      | 51:1:596:U:C5       | 3.04                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1:848:C:H2'     | 51:1:849:A:C8      | 2.51                     | 0.46              |
| 51:1:1509:A:H2'    | 51:1:1510:G:C8     | 2.49                     | 0.46              |
| 51:1:1768:C:H42    | 51:1:1984:G:H1     | 1.62                     | 0.46              |
| 51:1:1923:U:O2'    | 51:1:1924:C:H5'    | 2.16                     | 0.46              |
| 57:A1:35:PHE:HA    | 57:A1:38:THR:HG22  | 1.97                     | 0.46              |
| 58:B1:105:ILE:HD12 | 58:B1:242:LEU:CD2  | 2.44                     | 0.46              |
| 58:B1:128:LEU:HD21 | 58:B1:188:LEU:HB3  | 1.97                     | 0.46              |
| 62:NG:135:ARG:O    | 62:NG:178:VAL:HA   | 2.16                     | 0.46              |
| 63:5:34:G:H3'      | 63:5:35:A:C8       | 2.50                     | 0.46              |
| 2:B:31:LYS:HG2     | 51:1:2885:G:N2     | 2.31                     | 0.46              |
| 11:K:3:HIS:HA      | 11:K:65:GLU:HA     | 1.97                     | 0.46              |
| 11:K:10:VAL:HG23   | 11:K:58:HIS:HB3    | 1.97                     | 0.46              |
| 11:K:41:ASP:OD1    | 11:K:58:HIS:NE2    | 2.39                     | 0.46              |
| 16:P:124:LYS:HB3   | 26:Z:34:ARG:HB3    | 1.98                     | 0.46              |
| 23:W:33:THR:OG1    | 23:W:34:GLU:N      | 2.49                     | 0.46              |
| 29:d:132:LYS:HG2   | 29:d:136:GLN:HE22  | 1.81                     | 0.46              |
| 33:i:112:LYS:HD2   | 33:i:128:ILE:HD12  | 1.97                     | 0.46              |
| 51:1:28:A:O2'      | 51:1:29:U:H5'      | 2.16                     | 0.46              |
| 51:1:44:A:H2'      | 51:1:45:G:O4'      | 2.15                     | 0.46              |
| 51:1:637:A:C6      | 51:1:652:U:H4'     | 2.50                     | 0.46              |
| 51:1:688:U:H5'     | 51:1:1780:A:C2     | 2.51                     | 0.46              |
| 51:1:853:C:O2'     | 51:1:854:C:H5'     | 2.16                     | 0.46              |
| 51:1:1090:A:C2     | 51:1:1102:C:H1'    | 2.50                     | 0.46              |
| 51:1:1117:C:H2'    | 51:1:1118:C:C6     | 2.50                     | 0.46              |
| 51:1:1173:U:C6     | 51:1:1174:U:H1'    | 2.51                     | 0.46              |
| 51:1:1183:U:H2'    | 51:1:1184:U:H6     | 1.80                     | 0.46              |
| 51:1:1210:G:P      | 51:1:1212:G:H5'    | 2.56                     | 0.46              |
| 51:1:1572:A:H2'    | 51:1:1573:G:O4'    | 2.16                     | 0.46              |
| 51:1:2294:G:O2'    | 51:1:2295:C:H5'    | 2.15                     | 0.46              |
| 55:8:14:DC:H2'     | 55:8:15:DC:H6      | 1.79                     | 0.46              |
| 58:B1:209:ASN:HA   | 58:B1:214:ARG:NH2  | 2.30                     | 0.46              |
| 58:B1:352:ARG:CD   | 59:B2:1268:GLN:NE2 | 2.67                     | 0.46              |
| 22:V:10:ARG:NE     | 22:V:55:GLY:O      | 2.48                     | 0.46              |
| 27:b:131:MET:H     | 27:b:131:MET:HG2   | 1.57                     | 0.46              |
| 31:f:87:GLN:HB3    | 31:f:162:ARG:HG3   | 1.96                     | 0.46              |
| 34:j:2:LYS:HA      | 51:1:995:C:C4      | 2.50                     | 0.46              |
| 51:1:538:A:O2'     | 51:1:539:G:H5'     | 2.14                     | 0.46              |
| 51:1:1285:A:H2'    | 51:1:1286:A:H5'    | 1.96                     | 0.46              |
| 51:1:1574:C:H2'    | 51:1:1575:C:C6     | 2.50                     | 0.46              |
| 51:1:1927:A:H2'    | 51:1:1928:A:C8     | 2.50                     | 0.46              |
| 51:1:2247:A:H2'    | 51:1:2248:C:H6     | 1.81                     | 0.46              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 51:1:2329:U:H2'     | 51:1:2330:G:C8     | 2.51                     | 0.46              |
| 51:1:2642:G:O5'     | 51:1:2642:G:H8     | 1.98                     | 0.46              |
| 59:B2:517:GLN:HB3   | 59:B2:760:ASN:H    | 1.79                     | 0.46              |
| 59:B2:1286:THR:O    | 59:B2:1290:MET:HB2 | 2.14                     | 0.46              |
| 63:5:8:U:H2'        | 63:5:13:C:H41      | 1.81                     | 0.46              |
| 63:5:26:A:H61       | 63:5:44:G:H22      | 1.64                     | 0.46              |
| 4:D:12:ARG:NH1      | 51:1:465:G:OP1     | 2.49                     | 0.46              |
| 8:H:171:ARG:HG2     | 8:H:173:PRO:HD3    | 1.96                     | 0.46              |
| 27:b:1:ALA:N        | 27:b:19:VAL:O      | 2.41                     | 0.46              |
| 36:l:69:ARG:NH1     | 51:1:2406:A:C2     | 2.84                     | 0.46              |
| 51:1:1090:A:H61     | 51:1:1101:U:H3     | 1.62                     | 0.46              |
| 51:1:1105:U:H2'     | 51:1:1106:G:H8     | 1.80                     | 0.46              |
| 51:1:1863:G:H2'     | 51:1:1864:U:C6     | 2.51                     | 0.46              |
| 51:1:2836:U:H2'     | 51:1:2837:A:H8     | 1.81                     | 0.46              |
| 55:8:20:DA:H4'      | 59:B2:143:ARG:NH1  | 2.31                     | 0.46              |
| 57:A1:212:ASP:OD1   | 57:A1:212:ASP:N    | 2.48                     | 0.46              |
| 59:B2:230:PHE:HB2   | 59:B2:333:ILE:HB   | 1.97                     | 0.46              |
| 59:B2:318:SER:OG    | 59:B2:320:ASP:OD1  | 2.31                     | 0.46              |
| 59:B2:1002:LEU:HD21 | 59:B2:1007:LYS:HB2 | 1.98                     | 0.46              |
| 65:0:27:THR:HA      | 65:0:30:ILE:HD12   | 1.96                     | 0.46              |
| 65:0:648:GLU:H      | 65:0:648:GLU:HG3   | 1.57                     | 0.46              |
| 26:Z:29:ALA:O       | 26:Z:32:ARG:NH1    | 2.49                     | 0.46              |
| 33:i:79:LEU:HD21    | 33:i:105:LEU:HD21  | 1.96                     | 0.46              |
| 33:i:109:ALA:HA     | 33:i:112:LYS:HB2   | 1.98                     | 0.46              |
| 39:o:29:HIS:HB3     | 39:o:36:TYR:HB2    | 1.98                     | 0.46              |
| 40:p:52:ARG:HH21    | 51:1:2720:U:H5''   | 1.80                     | 0.46              |
| 51:1:290:U:O2'      | 51:1:291:G:H5'     | 2.16                     | 0.46              |
| 51:1:519:U:C2       | 51:1:520:G:C8      | 3.03                     | 0.46              |
| 51:1:1034:G:C5      | 51:1:1035:U:C4     | 3.04                     | 0.46              |
| 51:1:1520:U:H2'     | 51:1:1521:G:O4'    | 2.16                     | 0.46              |
| 51:1:1869:G:H3'     | 51:1:1870:C:C5'    | 2.38                     | 0.46              |
| 51:1:2679:A:O2'     | 51:1:2680:U:H5'    | 2.15                     | 0.46              |
| 51:1:2783:U:H2'     | 51:1:2784:U:C6     | 2.51                     | 0.46              |
| 51:1:2813:A:O2'     | 51:1:2814:A:H5'    | 2.15                     | 0.46              |
| 57:A2:294:ASN:HA    | 61:NA:464:ILE:N    | 2.28                     | 0.46              |
| 59:B2:735:LYS:HA    | 59:B2:748:ILE:HG22 | 1.97                     | 0.46              |
| 7:G:65:LYS:HE2      | 7:G:65:LYS:HB2     | 1.78                     | 0.46              |
| 9:I:114:ARG:HA      | 9:I:117:VAL:HG22   | 1.98                     | 0.46              |
| 15:O:100:ILE:O      | 62:NG:170:PRO:O    | 2.34                     | 0.46              |
| 31:f:106:LEU:O      | 31:f:151:ARG:NH2   | 2.37                     | 0.46              |
| 51:1:338:G:O2'      | 51:1:339:U:H5'     | 2.14                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1:409:G:H2'     | 51:1:410:G:C8      | 2.51                     | 0.46              |
| 51:1:438:G:O2'     | 51:1:439:A:H5'     | 2.16                     | 0.46              |
| 51:1:1710:G:H2'    | 51:1:1711:A:C8     | 2.51                     | 0.46              |
| 51:1:1930:G:O2'    | 51:1:1931:U:OP2    | 2.33                     | 0.46              |
| 51:1:2315:G:H2'    | 51:1:2316:G:H8     | 1.80                     | 0.46              |
| 51:1:2339:C:H2'    | 51:1:2340:A:H8     | 1.81                     | 0.46              |
| 57:A2:102:LEU:HD12 | 57:A2:115:ILE:HG12 | 1.96                     | 0.46              |
| 58:B1:198:CYS:HA   | 58:B1:221:ILE:CD1  | 2.45                     | 0.46              |
| 58:B1:772:TYR:HE2  | 59:B2:561:ILE:HG21 | 1.80                     | 0.46              |
| 58:B1:1167:LYS:NZ  | 58:B1:1170:LYS:HB2 | 2.30                     | 0.46              |
| 16:P:127:ARG:HB2   | 26:Z:34:ARG:HH22   | 1.81                     | 0.46              |
| 21:U:70:ARG:O      | 21:U:74:LEU:N      | 2.47                     | 0.46              |
| 22:V:11:VAL:HG13   | 22:V:58:VAL:HG21   | 1.98                     | 0.46              |
| 31:f:90:GLY:HA2    | 31:f:159:LYS:HG2   | 1.98                     | 0.46              |
| 51:1:342:A:H2'     | 51:1:343:C:O4'     | 2.16                     | 0.46              |
| 51:1:848:C:H2'     | 51:1:849:A:H8      | 1.80                     | 0.46              |
| 51:1:1486:U:O2'    | 51:1:1487:U:H5'    | 2.14                     | 0.46              |
| 55:8:13:DT:C6      | 58:B1:791:ALA:HA   | 2.51                     | 0.46              |
| 57:A1:231:PHE:O    | 57:A2:218:ARG:NH1  | 2.49                     | 0.46              |
| 58:B1:1219:ASP:O   | 58:B1:1223:LEU:HB2 | 2.15                     | 0.46              |
| 63:5:6:G:H2'       | 63:5:7:A:C8        | 2.51                     | 0.46              |
| 8:H:152:VAL:HG12   | 8:H:197:VAL:HG22   | 1.98                     | 0.45              |
| 12:L:142:ARG:HH21  | 64:6:42:G:H4'      | 1.81                     | 0.45              |
| 17:Q:45:ASN:ND2    | 17:Q:88:ASP:OD2    | 2.39                     | 0.45              |
| 28:c:170:VAL:HG21  | 51:1:2679:A:H5'    | 1.97                     | 0.45              |
| 29:d:32:VAL:HG21   | 36:l:6:LEU:HD13    | 1.99                     | 0.45              |
| 35:k:70:ARG:NH1    | 51:1:2684:U:O4'    | 2.49                     | 0.45              |
| 43:s:82:MET:HE1    | 51:1:1322:A:H5''   | 1.98                     | 0.45              |
| 51:1:360:U:H2'     | 51:1:361:G:H1'     | 1.98                     | 0.45              |
| 51:1:607:U:O4      | 51:1:620:G:H5'     | 2.17                     | 0.45              |
| 51:1:1170:C:H2'    | 51:1:1171:G:C8     | 2.51                     | 0.45              |
| 51:1:1381:G:H2'    | 51:1:1382:G:H5'    | 1.98                     | 0.45              |
| 51:1:2141:G:H1     | 51:1:2151:U:H3     | 1.63                     | 0.45              |
| 51:1:2648:G:C2     | 51:1:2649:C:C2     | 3.04                     | 0.45              |
| 59:B2:712:SER:OG   | 59:B2:713:GLY:N    | 2.49                     | 0.45              |
| 65:0:574:MET:HE1   | 65:0:601:PHE:CE2   | 2.50                     | 0.45              |
| 12:L:142:ARG:HA    | 12:L:145:GLU:HG3   | 1.97                     | 0.45              |
| 14:N:11:ARG:NH2    | 53:3:1347:G:O6     | 2.49                     | 0.45              |
| 17:Q:72:ASN:HD21   | 17:Q:103:CYS:HA    | 1.81                     | 0.45              |
| 31:f:1:SER:HA      | 51:1:2749:A:OP1    | 2.15                     | 0.45              |
| 35:k:5:GLN:NE2     | 51:1:1668:A:H5''   | 2.31                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:t:34:VAL:HG21   | 44:t:43:ILE:HD11   | 1.99                     | 0.45              |
| 47:w:37:ARG:HA     | 47:w:37:ARG:HD3    | 1.70                     | 0.45              |
| 51:1:6:A:H2'       | 51:1:7:G:C8        | 2.52                     | 0.45              |
| 51:1:466:A:C2'     | 51:1:467:G:H5'     | 2.46                     | 0.45              |
| 51:1:569:U:H1'     | 51:1:947:A:O4'     | 2.16                     | 0.45              |
| 51:1:1288:G:C5     | 51:1:1327:A:C2     | 3.04                     | 0.45              |
| 51:1:1550:C:O2'    | 51:1:1551:A:H5'    | 2.16                     | 0.45              |
| 51:1:2743:U:H2'    | 51:1:2744:G:O4'    | 2.16                     | 0.45              |
| 58:B1:375:GLU:O    | 59:B2:1247:SER:HB3 | 2.16                     | 0.45              |
| 60:W0:25:ARG:NH1   | 60:W0:61:ASN:OD1   | 2.49                     | 0.45              |
| 63:5:55:U:O2       | 63:5:57:G:H1'      | 2.17                     | 0.45              |
| 13:M:83:ARG:NH2    | 53:3:587:G:OP1     | 2.44                     | 0.45              |
| 18:R:16:ILE:O      | 18:R:19:THR:OG1    | 2.26                     | 0.45              |
| 33:i:106:GLN:OE1   | 33:i:125:THR:OG1   | 2.31                     | 0.45              |
| 34:j:108:MET:CE    | 51:1:1138:G:H21    | 2.29                     | 0.45              |
| 37:m:34:LYS:N      | 37:m:129:THR:O     | 2.47                     | 0.45              |
| 41:q:82:LEU:HD22   | 41:q:87:VAL:HB     | 1.98                     | 0.45              |
| 49:y:6:LEU:HD13    | 49:y:56:LEU:HD22   | 1.98                     | 0.45              |
| 51:1:1087:G:H22    | 51:1:1103:A:H1'    | 1.76                     | 0.45              |
| 51:1:1287:A:O2'    | 51:1:1288:G:H5'    | 2.15                     | 0.45              |
| 51:1:1488:C:H2'    | 51:1:1489:C:C6     | 2.51                     | 0.45              |
| 51:1:2661:G:O2'    | 51:1:2662:A:H5'    | 2.16                     | 0.45              |
| 57:A2:80:GLU:HG3   | 59:B2:694:ARG:HH22 | 1.81                     | 0.45              |
| 58:B1:201:LEU:HD11 | 58:B1:220:ARG:NH1  | 2.32                     | 0.45              |
| 58:B1:515:ARG:NH2  | 58:B1:718:SER:O    | 2.48                     | 0.45              |
| 64:6:7:G:H3'       | 64:6:49:G:OP2      | 2.16                     | 0.45              |
| 7:G:166:ASP:HB3    | 7:G:190:SER:HB2    | 1.98                     | 0.45              |
| 18:R:97:ARG:HB2    | 18:R:99:GLN:HE22   | 1.81                     | 0.45              |
| 28:c:4:LEU:HD11    | 28:c:100:LEU:HD21  | 1.98                     | 0.45              |
| 48:x:30:PRO:HG2    | 48:x:32:LEU:HD11   | 1.98                     | 0.45              |
| 51:1:30:G:H2'      | 51:1:31:C:O4'      | 2.17                     | 0.45              |
| 51:1:438:G:H2'     | 51:1:439:A:C8      | 2.51                     | 0.45              |
| 51:1:1605:C:H2'    | 51:1:1606:C:H5'    | 1.98                     | 0.45              |
| 53:3:1200:C:H5''   | 53:3:1201:A:H3'    | 1.97                     | 0.45              |
| 53:3:1383:C:H4'    | 64:6:35:A:H2       | 1.81                     | 0.45              |
| 55:8:1:DC:H2''     | 55:8:2:DC:C6       | 2.51                     | 0.45              |
| 58:B1:67:ASP:OD1   | 58:B1:67:ASP:O     | 2.35                     | 0.45              |
| 58:B1:115:TRP:HB3  | 58:B1:1333:THR:CG2 | 2.46                     | 0.45              |
| 59:B2:24:VAL:HG11  | 59:B2:704:MET:HE1  | 1.99                     | 0.45              |
| 7:G:8:MET:HE3      | 7:G:8:MET:HB3      | 1.84                     | 0.45              |
| 7:G:142:LYS:NZ     | 53:3:1098:C:OP1    | 2.49                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 7:G:172:ILE:O      | 7:G:176:ASN:ND2     | 2.50                     | 0.45              |
| 10:J:101:GLY:H     | 10:J:121:ASN:HB3    | 1.82                     | 0.45              |
| 12:L:70:PRO:HG3    | 12:L:98:LEU:HD23    | 1.97                     | 0.45              |
| 19:S:58:ARG:HH21   | 53:3:980:C:H4'      | 1.81                     | 0.45              |
| 51:1:1049:C:C2'    | 51:1:1050:A:H5'     | 2.47                     | 0.45              |
| 51:1:1140:C:C2'    | 51:1:1141:U:H5'     | 2.47                     | 0.45              |
| 51:1:1140:C:H2'    | 51:1:1141:U:H5'     | 1.97                     | 0.45              |
| 51:1:1239:G:O2'    | 51:1:1240:U:H5'     | 2.17                     | 0.45              |
| 51:1:1866:A:H2'    | 51:1:1867:G:O4'     | 2.16                     | 0.45              |
| 51:1:1952:A:H2'    | 51:1:1953:A:C8      | 2.51                     | 0.45              |
| 51:1:2314:A:H2'    | 51:1:2315:G:H8      | 1.78                     | 0.45              |
| 51:1:2364:C:O2'    | 51:1:2365:G:H5'     | 2.17                     | 0.45              |
| 51:1:2528:U:O2'    | 51:1:2529:G:H3'     | 2.16                     | 0.45              |
| 51:1:2741:A:H2'    | 51:1:2742:G:H5'     | 1.98                     | 0.45              |
| 53:3:618:C:N4      | 53:3:621:A:OP2      | 2.49                     | 0.45              |
| 58:B1:842:ARG:HH22 | 58:B1:1250:ASP:HB2  | 1.80                     | 0.45              |
| 58:B1:1158:GLU:HA  | 58:B1:1223:LEU:HD21 | 1.99                     | 0.45              |
| 11:K:75:GLU:O      | 11:K:79:ARG:N       | 2.47                     | 0.45              |
| 29:d:136:GLN:HA    | 29:d:139:LYS:HE2    | 1.99                     | 0.45              |
| 35:k:121:GLU:HG2   | 35:k:122:VAL:HG23   | 1.97                     | 0.45              |
| 45:u:32:LYS:HG2    | 45:u:65:GLN:HA      | 1.99                     | 0.45              |
| 51:1:540:C:O2'     | 51:1:541:A:H5'      | 2.16                     | 0.45              |
| 51:1:707:G:C2'     | 51:1:708:G:H5'      | 2.47                     | 0.45              |
| 51:1:1324:G:O2'    | 51:1:1326:U:OP2     | 2.29                     | 0.45              |
| 51:1:1412:U:H2'    | 51:1:1413:A:H8      | 1.81                     | 0.45              |
| 51:1:1868:C:H2'    | 51:1:1869:G:C8      | 2.52                     | 0.45              |
| 51:1:2030:A:N3     | 51:1:2499:C:H5''    | 2.31                     | 0.45              |
| 51:1:2849:U:H4'    | 51:1:2868:A:C2      | 2.51                     | 0.45              |
| 53:3:765:G:H1      | 53:3:812:G:HO2'     | 1.63                     | 0.45              |
| 53:3:1376:U:H2'    | 53:3:1377:A:C8      | 2.52                     | 0.45              |
| 58:B1:395:LYS:HZ2  | 58:B1:399:LYS:CE    | 2.28                     | 0.45              |
| 2:B:4:GLN:HG3      | 51:1:2054:A:C2      | 2.52                     | 0.45              |
| 8:H:5:HIS:CE1      | 8:H:7:ASN:HB3       | 2.51                     | 0.45              |
| 9:I:13:ARG:NH1     | 53:3:542:G:O3'      | 2.50                     | 0.45              |
| 12:L:137:ARG:NH1   | 12:L:138:GLU:OE2    | 2.48                     | 0.45              |
| 27:b:257:ARG:HH22  | 27:b:262:THR:HG1    | 1.62                     | 0.45              |
| 41:q:111:LYS:HA    | 41:q:111:LYS:HD2    | 1.81                     | 0.45              |
| 51:1:111:A:O2'     | 51:1:112:U:H5'      | 2.17                     | 0.45              |
| 51:1:167:A:H2'     | 51:1:168:G:O4'      | 2.16                     | 0.45              |
| 51:1:893:C:H2'     | 51:1:894:U:O4'      | 2.17                     | 0.45              |
| 51:1:1766:G:C2'    | 51:1:1767:G:H5'     | 2.45                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:1:2636:C:O2'    | 51:1:2637:U:H5'     | 2.16                     | 0.45              |
| 51:1:2651:C:H2'    | 51:1:2652:C:H6      | 1.81                     | 0.45              |
| 54:4:44:G:OP1      | 59:B2:1073:LYS:NZ   | 2.35                     | 0.45              |
| 58:B1:128:LEU:CD2  | 58:B1:188:LEU:HB3   | 2.47                     | 0.45              |
| 58:B1:213:LYS:CA   | 58:B1:213:LYS:HE3   | 2.47                     | 0.45              |
| 58:B1:343:LEU:HD11 | 58:B1:1324:SER:HB3  | 1.98                     | 0.45              |
| 58:B1:478:LEU:HD21 | 60:W0:47:THR:HG23   | 1.99                     | 0.45              |
| 59:B2:674:ASP:OD2  | 59:B2:1070:HIS:ND1  | 2.50                     | 0.45              |
| 59:B2:900:LYS:HE3  | 59:B2:900:LYS:HB3   | 1.62                     | 0.45              |
| 63:5:22:G:H2'      | 63:5:23:A:C8        | 2.52                     | 0.45              |
| 65:0:473:MET:HE3   | 65:0:473:MET:HB3    | 1.87                     | 0.45              |
| 2:B:8:THR:OG1      | 2:B:9:ARG:N         | 2.49                     | 0.45              |
| 9:I:173:ASP:HB3    | 9:I:178:GLU:HB3     | 1.98                     | 0.45              |
| 17:Q:23:LEU:HD12   | 17:Q:29:LYS:HD2     | 1.97                     | 0.45              |
| 45:u:12:VAL:HA     | 45:u:69:VAL:HG12    | 1.99                     | 0.45              |
| 51:1:395:U:H2'     | 51:1:396:G:C8       | 2.52                     | 0.45              |
| 51:1:1071:G:HO2'   | 51:1:1089:A:H2'     | 1.81                     | 0.45              |
| 51:1:1710:G:O2'    | 51:1:1711:A:H5'     | 2.17                     | 0.45              |
| 51:1:2047:C:O2'    | 51:1:2048:G:H5'     | 2.16                     | 0.45              |
| 51:1:2717:C:N3     | 51:1:2718:G:N7      | 2.65                     | 0.45              |
| 58:B1:484:MET:CE   | 59:B2:1278:LEU:HD21 | 2.46                     | 0.45              |
| 59:B2:557:ARG:NH2  | 59:B2:607:SER:O     | 2.49                     | 0.45              |
| 9:I:120:LYS:HG2    | 9:I:130:ASN:HB3     | 1.99                     | 0.45              |
| 15:O:29:ALA:HB2    | 15:O:87:LEU:HD11    | 1.99                     | 0.45              |
| 28:c:106:LYS:HA    | 28:c:176:ASP:HA     | 1.99                     | 0.45              |
| 33:i:49:GLU:OE1    | 33:i:81:LYS:NZ      | 2.41                     | 0.45              |
| 51:1:195:A:H3'     | 51:1:196:A:H4'      | 1.99                     | 0.45              |
| 51:1:367:G:O2'     | 51:1:368:A:H5'      | 2.17                     | 0.45              |
| 51:1:432:A:O2'     | 51:1:433:C:H5'      | 2.17                     | 0.45              |
| 51:1:500:G:N2      | 51:1:502:A:H3'      | 2.32                     | 0.45              |
| 51:1:854:C:H2'     | 51:1:855:G:C8       | 2.52                     | 0.45              |
| 51:1:1344:U:H3'    | 51:1:1345:C:H5'     | 1.97                     | 0.45              |
| 51:1:1832:C:O5'    | 51:1:1832:C:H6      | 2.00                     | 0.45              |
| 51:1:1882:U:O2'    | 51:1:1883:U:H5'     | 2.17                     | 0.45              |
| 51:1:2085:U:O2'    | 51:1:2086:U:H5'     | 2.16                     | 0.45              |
| 51:1:2626:C:H2'    | 51:1:2627:G:C8      | 2.51                     | 0.45              |
| 53:3:477:C:H2'     | 53:3:478:A:C8       | 2.52                     | 0.45              |
| 55:8:16:DT:H2'     | 55:8:17:DC:C6       | 2.52                     | 0.45              |
| 58:B1:76:LYS:NZ    | 58:B1:76:LYS:HB3    | 2.32                     | 0.45              |
| 58:B1:211:GLU:CG   | 58:B1:215:LYS:HE3   | 2.44                     | 0.45              |
| 58:B1:472:LEU:CD1  | 59:B2:1294:LYS:HG2  | 2.47                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 58:B1:926:PRO:HB2   | 58:B1:1241:TYR:HE1 | 1.82                     | 0.45              |
| 59:B2:1314:GLN:HA   | 60:W0:28:ARG:HH22  | 1.80                     | 0.45              |
| 9:I:1:ALA:N         | 53:3:405:U:O4      | 2.45                     | 0.45              |
| 11:K:5:GLU:HB2      | 11:K:90:MET:HB2    | 1.98                     | 0.45              |
| 33:i:8:VAL:HG11     | 33:i:26:ALA:HB2    | 1.98                     | 0.45              |
| 51:1:974:G:H1'      | 51:1:975:A:C8      | 2.52                     | 0.45              |
| 51:1:1020:A:C2      | 51:1:1141:U:C2     | 3.05                     | 0.45              |
| 51:1:1338:G:H2'     | 51:1:1339:G:C8     | 2.51                     | 0.45              |
| 51:1:1915:U:O2      | 51:1:1915:U:O4'    | 2.34                     | 0.45              |
| 51:1:2137:U:H2'     | 51:1:2138:G:C8     | 2.50                     | 0.45              |
| 51:1:2700:A:O2'     | 51:1:2701:U:H5'    | 2.17                     | 0.45              |
| 51:1:2844:G:H2'     | 51:1:2845:U:O4'    | 2.16                     | 0.45              |
| 53:3:647:C:H2'      | 53:3:648:A:H8      | 1.81                     | 0.45              |
| 58:B1:33:TRP:HZ2    | 59:B2:1336:ASN:OD1 | 2.00                     | 0.45              |
| 58:B1:68:TYR:O      | 58:B1:75:TYR:CD2   | 2.70                     | 0.45              |
| 58:B1:109:SER:HB2   | 58:B1:296:LYS:HG2  | 1.98                     | 0.45              |
| 58:B1:395:LYS:NZ    | 58:B1:399:LYS:CD   | 2.74                     | 0.45              |
| 59:B2:176:ILE:HD11  | 59:B2:428:VAL:HG21 | 1.98                     | 0.45              |
| 7:G:26:MET:HE1      | 7:G:186:VAL:HB     | 1.99                     | 0.44              |
| 7:G:33:ALA:HB3      | 7:G:37:VAL:HG12    | 1.99                     | 0.44              |
| 7:G:65:LYS:HG2      | 7:G:153:MET:HG3    | 1.98                     | 0.44              |
| 10:J:110:MET:HE3    | 10:J:110:MET:HB2   | 1.79                     | 0.44              |
| 18:R:107:THR:OG1    | 53:3:947:G:O3'     | 2.35                     | 0.44              |
| 21:U:79:ASN:HB2     | 21:U:82:ALA:HB3    | 1.99                     | 0.44              |
| 28:c:151:THR:O      | 51:1:1130:U:C4     | 2.70                     | 0.44              |
| 33:i:135:MET:CE     | 51:1:1062:G:H21    | 2.30                     | 0.44              |
| 40:p:88:ARG:HH11    | 40:p:114:ASN:HD21  | 1.65                     | 0.44              |
| 51:1:545:U:O2       | 51:1:546:U:H1'     | 2.17                     | 0.44              |
| 51:1:1749:A:H2'     | 51:1:1750:G:H8     | 1.82                     | 0.44              |
| 51:1:1800:C:O2      | 51:1:1802:A:C8     | 2.70                     | 0.44              |
| 51:1:2122:U:H2'     | 51:1:2123:G:O4'    | 2.17                     | 0.44              |
| 51:1:2402:U:O2'     | 51:1:2403:C:H3'    | 2.17                     | 0.44              |
| 51:1:2889:C:O2'     | 51:1:2890:G:H5'    | 2.17                     | 0.44              |
| 53:3:112:G:N2       | 53:3:354:G:O5'     | 2.49                     | 0.44              |
| 53:3:1253:G:H2'     | 53:3:1254:A:C8     | 2.52                     | 0.44              |
| 58:B1:201:LEU:CB    | 58:B1:221:ILE:HD13 | 2.47                     | 0.44              |
| 58:B1:395:LYS:NZ    | 58:B1:399:LYS:HE2  | 2.32                     | 0.44              |
| 58:B1:770:LEU:HD13  | 59:B2:618:GLN:CD   | 2.42                     | 0.44              |
| 58:B1:804:ALA:HB2   | 58:B1:1256:ILE:CD1 | 2.48                     | 0.44              |
| 58:B1:1357:ILE:HG22 | 58:B1:1359:ALA:H   | 1.82                     | 0.44              |
| 7:G:173:LYS:HE3     | 7:G:173:LYS:HB2    | 1.76                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:H:134:LYS:HG2     | 8:H:138:GLN:HE21    | 1.82                     | 0.44              |
| 51:1:208:C:O2'      | 51:1:209:C:H5'      | 2.18                     | 0.44              |
| 51:1:354:A:H2'      | 51:1:355:U:O4'      | 2.17                     | 0.44              |
| 51:1:696:G:H2'      | 51:1:697:G:O4'      | 2.18                     | 0.44              |
| 51:1:1747:U:H2'     | 51:1:1748:C:C6      | 2.53                     | 0.44              |
| 51:1:1807:G:H2'     | 51:1:1808:A:C5'     | 2.30                     | 0.44              |
| 51:1:2658:C:H2'     | 51:1:2659:G:O4'     | 2.16                     | 0.44              |
| 51:1:2869:G:H2'     | 51:1:2870:C:O4'     | 2.17                     | 0.44              |
| 53:3:146:G:N2       | 53:3:177:G:N7       | 2.66                     | 0.44              |
| 53:3:1498:U:H4'     | 53:3:1519:A:H2      | 1.82                     | 0.44              |
| 58:B1:201:LEU:CD1   | 58:B1:224:LEU:HD12  | 2.47                     | 0.44              |
| 58:B1:1227:HIS:HA   | 58:B1:1230:THR:HG22 | 1.99                     | 0.44              |
| 59:B2:998:LEU:HG    | 59:B2:1011:LEU:HB3  | 1.99                     | 0.44              |
| 14:N:104:THR:HG23   | 53:3:1180:A:H5'     | 1.99                     | 0.44              |
| 18:R:1:ALA:HB3      | 18:R:56:ARG:HH22    | 1.82                     | 0.44              |
| 29:d:68:ALA:HA      | 51:1:1255:U:C6      | 2.52                     | 0.44              |
| 34:j:34:ARG:NH2     | 34:j:39:LYS:O       | 2.51                     | 0.44              |
| 38:n:65:LEU:HD11    | 51:1:2870:C:H5''    | 1.99                     | 0.44              |
| 45:u:17:ASP:HA      | 45:u:20:LYS:HE2     | 2.00                     | 0.44              |
| 51:1:239:C:H2'      | 51:1:240:C:O4'      | 2.16                     | 0.44              |
| 51:1:355:U:H6       | 51:1:355:U:O5'      | 1.99                     | 0.44              |
| 51:1:639:U:H2'      | 51:1:640:C:C6       | 2.52                     | 0.44              |
| 51:1:654:A:N3       | 51:1:654:A:H5''     | 2.31                     | 0.44              |
| 51:1:1680:U:C2'     | 51:1:1681:G:H5'     | 2.47                     | 0.44              |
| 51:1:1922:G:H2'     | 51:1:1923:U:O4'     | 2.18                     | 0.44              |
| 51:1:2101:A:H2'     | 51:1:2102:G:H8      | 1.81                     | 0.44              |
| 51:1:2201:G:H2'     | 51:1:2202:U:O4'     | 2.17                     | 0.44              |
| 51:1:2805:C:O2'     | 51:1:2806:C:H5'     | 2.18                     | 0.44              |
| 52:2:66:A:H4'       | 52:2:67:G:C8        | 2.53                     | 0.44              |
| 57:A1:185:TYR:HA    | 57:A1:202:VAL:O     | 2.16                     | 0.44              |
| 59:B2:1246:ARG:HH11 | 59:B2:1266:GLY:HA2  | 1.82                     | 0.44              |
| 64:6:11:A:H2'       | 64:6:12:G:C8        | 2.52                     | 0.44              |
| 6:F:8:LYS:NZ        | 51:1:2467:C:OP1     | 2.37                     | 0.44              |
| 9:I:47:LEU:HD23     | 9:I:47:LEU:HA       | 1.85                     | 0.44              |
| 11:K:62:MET:HB3     | 11:K:64:VAL:HG13    | 1.98                     | 0.44              |
| 31:f:132:LEU:HB3    | 31:f:140:ILE:HD11   | 1.99                     | 0.44              |
| 51:1:150:U:H2'      | 51:1:151:C:C6       | 2.52                     | 0.44              |
| 51:1:720:U:H2'      | 51:1:721:A:H8       | 1.82                     | 0.44              |
| 51:1:1500:G:O2'     | 51:1:1501:G:H5'     | 2.16                     | 0.44              |
| 51:1:2236:U:H2'     | 51:1:2237:G:C5'     | 2.46                     | 0.44              |
| 58:B1:141:PHE:CE2   | 58:B1:296:LYS:CB    | 2.94                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 58:B1:245:LEU:CG   | 58:B1:246:PRO:HD2 | 2.47                     | 0.44              |
| 58:B1:385:LEU:HD23 | 58:B1:390:LEU:HB2 | 1.98                     | 0.44              |
| 58:B1:388:ARG:HG2  | 58:B1:388:ARG:NH1 | 2.32                     | 0.44              |
| 65:0:370:LYS:HE3   | 65:0:370:LYS:HB3  | 1.82                     | 0.44              |
| 14:N:119:LYS:NZ    | 53:3:1350:A:N7    | 2.64                     | 0.44              |
| 28:c:150:GLN:HE22  | 51:1:2032:G:H1'   | 1.82                     | 0.44              |
| 33:i:9:LYS:HD2     | 51:1:1061:U:OP1   | 2.18                     | 0.44              |
| 48:x:51:SER:OG     | 48:x:54:GLY:N     | 2.48                     | 0.44              |
| 51:1:293:U:H2'     | 51:1:294:A:H5''   | 1.99                     | 0.44              |
| 51:1:704:G:H1'     | 51:1:727:A:H62    | 1.83                     | 0.44              |
| 51:1:1280:G:C2'    | 51:1:1281:G:H5'   | 2.46                     | 0.44              |
| 51:1:1465:G:O2'    | 51:1:1466:U:H5'   | 2.17                     | 0.44              |
| 51:1:1670:C:O2'    | 51:1:1671:U:H5'   | 2.16                     | 0.44              |
| 51:1:1672:A:N3     | 51:1:2582:G:H5'   | 2.27                     | 0.44              |
| 51:1:2204:G:H2'    | 51:1:2205:A:H8    | 1.81                     | 0.44              |
| 58:B1:75:TYR:CD2   | 58:B1:75:TYR:O    | 2.70                     | 0.44              |
| 58:B1:375:GLU:HB3  | 59:B2:1245:ALA:CB | 2.48                     | 0.44              |
| 58:B1:506:VAL:HG23 | 58:B1:628:GLY:HA3 | 1.99                     | 0.44              |
| 8:H:37:LYS:HD3     | 8:H:37:LYS:HA     | 1.81                     | 0.44              |
| 14:N:74:GLN:OE1    | 53:3:1249:C:O2'   | 2.35                     | 0.44              |
| 29:d:188:MET:HB2   | 29:d:192:ALA:HB3  | 1.99                     | 0.44              |
| 30:e:71:LYS:HA     | 30:e:71:LYS:HD2   | 1.79                     | 0.44              |
| 47:w:12:SER:OG     | 47:w:13:GLU:N     | 2.51                     | 0.44              |
| 49:y:20:ASN:HA     | 49:y:23:ARG:HB2   | 1.99                     | 0.44              |
| 51:1:29:U:O5'      | 51:1:29:U:H6      | 2.00                     | 0.44              |
| 51:1:336:C:O2'     | 51:1:337:C:H5'    | 2.18                     | 0.44              |
| 63:5:49:C:H2'      | 63:5:50:U:C6      | 2.52                     | 0.44              |
| 19:S:44:VAL:O      | 19:S:48:GLN:NE2   | 2.50                     | 0.44              |
| 33:i:131:THR:HB    | 51:1:1060:U:O4    | 2.18                     | 0.44              |
| 41:q:47:ARG:NH2    | 41:q:51:GLN:OE1   | 2.51                     | 0.44              |
| 51:1:163:C:O2'     | 51:1:164:C:H5'    | 2.17                     | 0.44              |
| 51:1:350:G:H2'     | 51:1:351:C:O4'    | 2.18                     | 0.44              |
| 51:1:518:G:O2'     | 51:1:519:U:H5'    | 2.18                     | 0.44              |
| 51:1:648:G:H2'     | 51:1:649:G:H8     | 1.83                     | 0.44              |
| 51:1:721:A:H2'     | 51:1:722:A:C8     | 2.53                     | 0.44              |
| 51:1:940:G:H3'     | 51:1:941:A:H5''   | 1.97                     | 0.44              |
| 51:1:1010:A:H1'    | 51:1:1153:C:H1'   | 2.00                     | 0.44              |
| 51:1:1199:U:H2'    | 51:1:1200:C:C6    | 2.52                     | 0.44              |
| 51:1:1507:C:H2'    | 51:1:1508:A:H4'   | 1.99                     | 0.44              |
| 51:1:1717:A:C2     | 51:1:1718:G:H1'   | 2.53                     | 0.44              |
| 51:1:2880:C:H2'    | 51:1:2880:C:O2    | 2.17                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 53:3:490:C:H2'     | 53:3:491:G:C8       | 2.53                     | 0.44              |
| 58:B1:894:VAL:HG22 | 58:B1:1258:ARG:HH11 | 1.83                     | 0.44              |
| 4:D:12:ARG:HH12    | 51:1:465:G:P        | 2.41                     | 0.44              |
| 10:J:24:VAL:HG23   | 10:J:26:GLY:H       | 1.82                     | 0.44              |
| 25:Y:49:ALA:HA     | 25:Y:52:GLU:HG3     | 2.00                     | 0.44              |
| 32:g:28:ASN:ND2    | 51:1:2092:U:OP2     | 2.36                     | 0.44              |
| 34:j:85:LYS:NZ     | 51:1:2768:U:OP1     | 2.49                     | 0.44              |
| 51:1:12:U:O2       | 51:1:12:U:H2'       | 2.18                     | 0.44              |
| 51:1:28:A:H2'      | 51:1:29:U:C6        | 2.53                     | 0.44              |
| 51:1:169:G:O2'     | 51:1:170:U:H5'      | 2.18                     | 0.44              |
| 51:1:859:G:HO2'    | 51:1:860:U:P        | 2.41                     | 0.44              |
| 51:1:1539:U:H2'    | 51:1:1540:G:C8      | 2.53                     | 0.44              |
| 52:2:39:A:O2'      | 52:2:46:A:N1        | 2.46                     | 0.44              |
| 53:3:75:G:H2'      | 53:3:76:G:C8        | 2.53                     | 0.44              |
| 53:3:1013:G:N2     | 53:3:1016:A:OP2     | 2.35                     | 0.44              |
| 57:A1:78:ILE:HA    | 57:A1:81:ILE:HG22   | 2.00                     | 0.44              |
| 58:B1:282:LEU:HA   | 58:B1:282:LEU:HD12  | 1.79                     | 0.44              |
| 65:0:580:PHE:HD2   | 65:0:581:GLY:N      | 2.16                     | 0.44              |
| 9:I:85:THR:HA      | 9:I:88:ASN:HB2      | 2.00                     | 0.44              |
| 17:Q:3:VAL:HA      | 17:Q:6:LEU:HD12     | 2.00                     | 0.44              |
| 24:X:76:THR:OG1    | 24:X:77:ARG:N       | 2.51                     | 0.44              |
| 25:Y:67:HIS:O      | 25:Y:69:ASN:ND2     | 2.51                     | 0.44              |
| 29:d:147:LEU:HD11  | 29:d:170:ARG:HG2    | 1.98                     | 0.44              |
| 30:e:122:ASP:OD2   | 30:e:126:ASN:ND2    | 2.42                     | 0.44              |
| 36:l:95:LEU:HD22   | 36:l:100:ILE:HD11   | 2.00                     | 0.44              |
| 49:y:19:LEU:HA     | 49:y:19:LEU:HD23    | 1.86                     | 0.44              |
| 51:1:161:A:C5      | 51:1:162:U:H5       | 2.36                     | 0.44              |
| 51:1:684:G:C2      | 51:1:794:A:C2       | 3.06                     | 0.44              |
| 51:1:1383:A:H2     | 51:1:1406:U:H1'     | 1.83                     | 0.44              |
| 51:1:1507:C:H2'    | 51:1:1508:A:O4'     | 2.18                     | 0.44              |
| 51:1:1625:C:H2'    | 51:1:1626:A:O4'     | 2.18                     | 0.44              |
| 51:1:2312:U:O2'    | 51:1:2313:C:H5'     | 2.17                     | 0.44              |
| 51:1:2411:A:H2'    | 51:1:2412:A:C8      | 2.53                     | 0.44              |
| 53:3:162:A:C5      | 53:3:163:C:H1'      | 2.53                     | 0.44              |
| 53:3:958:A:N3      | 53:3:985:C:O2'      | 2.48                     | 0.44              |
| 58:B1:1033:GLY:HA3 | 58:B1:1081:VAL:O    | 2.18                     | 0.44              |
| 59:B2:805:MET:HE3  | 59:B2:805:MET:HB2   | 1.86                     | 0.44              |
| 59:B2:811:ASN:ND2  | 59:B2:1098:LEU:O    | 2.51                     | 0.44              |
| 60:W0:58:LEU:HD12  | 60:W0:59:ILE:HG12   | 2.00                     | 0.44              |
| 63:5:69:G:H2'      | 63:5:70:G:C8        | 2.52                     | 0.44              |
| 7:G:67:LEU:HD21    | 7:G:91:VAL:HG23     | 2.00                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 15:O:88:MET:HE3    | 15:O:88:MET:HB3     | 1.70                     | 0.43              |
| 18:R:43:LYS:HB2    | 18:R:46:GLU:HG2     | 1.99                     | 0.43              |
| 42:r:19:THR:OG1    | 42:r:95:ASP:OD1     | 2.35                     | 0.43              |
| 46:v:62:THR:O      | 46:v:62:THR:OG1     | 2.35                     | 0.43              |
| 50:z:30:ARG:HG2    | 50:z:33:HIS:HB2     | 1.99                     | 0.43              |
| 50:z:37:ARG:HA     | 50:z:37:ARG:HD3     | 1.83                     | 0.43              |
| 50:z:38:GLU:CD     | 51:1:928:A:H5'      | 2.43                     | 0.43              |
| 51:1:192:C:H2'     | 51:1:193:U:H5'      | 1.99                     | 0.43              |
| 51:1:1452:G:H2'    | 51:1:1453:A:OP2     | 2.17                     | 0.43              |
| 51:1:1565:C:C5     | 51:1:1567:G:C6      | 3.06                     | 0.43              |
| 53:3:908:A:H2'     | 53:3:909:A:H8       | 1.83                     | 0.43              |
| 58:B1:1026:PRO:HB2 | 58:B1:1028:ILE:HG23 | 2.00                     | 0.43              |
| 59:B2:538:LEU:HD13 | 59:B2:543:ALA:HB2   | 2.00                     | 0.43              |
| 62:NG:161:SER:CB   | 62:NG:170:PRO:HA    | 2.47                     | 0.43              |
| 8:H:134:LYS:HB3    | 8:H:134:LYS:HE2     | 1.84                     | 0.43              |
| 11:K:38:ARG:HH11   | 11:K:61:LEU:HD21    | 1.83                     | 0.43              |
| 12:L:113:LYS:HB3   | 53:3:1297:G:H21     | 1.82                     | 0.43              |
| 14:N:105:ARG:NH1   | 14:N:109:GLN:OE1    | 2.49                     | 0.43              |
| 30:e:171:ALA:C     | 30:e:173:ASP:H      | 2.26                     | 0.43              |
| 33:i:123:ALA:HB1   | 51:1:1081:U:H4'     | 2.00                     | 0.43              |
| 35:k:38:ILE:HG22   | 35:k:61:VAL:HB      | 2.01                     | 0.43              |
| 42:r:80:ARG:HD3    | 51:1:566:U:O4       | 2.17                     | 0.43              |
| 51:1:43:G:H2'      | 51:1:44:A:C8        | 2.53                     | 0.43              |
| 51:1:107:G:H2'     | 51:1:108:G:H8       | 1.82                     | 0.43              |
| 51:1:198:C:N4      | 51:1:248:G:H1       | 2.14                     | 0.43              |
| 51:1:819:A:H5'     | 51:1:973:A:N1       | 2.33                     | 0.43              |
| 51:1:1571:A:H2'    | 51:1:1572:A:C8      | 2.54                     | 0.43              |
| 51:1:2241:A:H2'    | 51:1:2242:G:H8      | 1.82                     | 0.43              |
| 53:3:1053:G:H4'    | 53:3:1054:C:H3'     | 2.00                     | 0.43              |
| 58:B1:161:THR:H    | 58:B1:164:GLN:HB2   | 1.82                     | 0.43              |
| 63:5:63:G:H2'      | 63:5:64:A:C8        | 2.53                     | 0.43              |
| 2:B:8:THR:HG23     | 2:B:11:LYS:H        | 1.81                     | 0.43              |
| 8:H:51:VAL:HA      | 8:H:69:THR:HG22     | 2.01                     | 0.43              |
| 10:J:104:ILE:HD11  | 10:J:114:LEU:HD13   | 1.99                     | 0.43              |
| 22:V:44:HIS:HB3    | 22:V:70:LYS:HG2     | 1.99                     | 0.43              |
| 25:Y:14:GLU:OE1    | 25:Y:17:ARG:NH2     | 2.51                     | 0.43              |
| 34:j:51:GLY:HA3    | 34:j:121:LYS:HE2    | 2.00                     | 0.43              |
| 51:1:30:G:O2'      | 51:1:31:C:H5'       | 2.17                     | 0.43              |
| 51:1:108:G:O2'     | 51:1:109:C:H5'      | 2.18                     | 0.43              |
| 51:1:150:U:O2'     | 51:1:151:C:H5'      | 2.18                     | 0.43              |
| 51:1:388:G:N7      | 51:1:390:U:H2'      | 2.33                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:1:1049:C:H2'   | 51:1:1050:A:H5'    | 2.00                     | 0.43              |
| 51:1:2152:G:N3    | 51:1:2152:G:H2'    | 2.33                     | 0.43              |
| 51:1:2285:C:C2'   | 51:1:2286:G:H5'    | 2.48                     | 0.43              |
| 51:1:2834:G:C2'   | 51:1:2835:A:H5'    | 2.49                     | 0.43              |
| 58:B1:287:ALA:HB1 | 58:B1:288:PRO:HD2  | 1.99                     | 0.43              |
| 58:B1:731:ARG:HB3 | 59:B2:1105:SER:HB2 | 2.00                     | 0.43              |
| 58:B1:847:ASP:N   | 58:B1:847:ASP:OD1  | 2.49                     | 0.43              |
| 58:B1:978:ARG:HD3 | 58:B1:999:TYR:H    | 1.83                     | 0.43              |
| 59:B2:800:MET:HE3 | 59:B2:800:MET:HB2  | 1.69                     | 0.43              |
| 21:U:31:ARG:HB2   | 53:3:310:G:H5''    | 2.01                     | 0.43              |
| 27:b:140:VAL:HG12 | 27:b:191:LEU:HD23  | 2.01                     | 0.43              |
| 51:1:1232:G:H2'   | 51:1:1233:C:C6     | 2.53                     | 0.43              |
| 51:1:1739:A:H2'   | 51:1:1740:G:O4'    | 2.19                     | 0.43              |
| 51:1:2671:G:C2    | 51:1:2672:U:C2     | 3.06                     | 0.43              |
| 58:B1:213:LYS:HE3 | 58:B1:213:LYS:HA   | 1.99                     | 0.43              |
| 63:5:13:C:H42     | 63:5:46:G:N2       | 2.16                     | 0.43              |
| 2:B:4:GLN:NE2     | 51:1:2056:G:O2'    | 2.52                     | 0.43              |
| 9:I:152:SER:HB3   | 53:3:436:C:H4'     | 2.00                     | 0.43              |
| 17:Q:72:ASN:OD1   | 17:Q:72:ASN:N      | 2.50                     | 0.43              |
| 18:R:104:ASN:HB3  | 18:R:105:ALA:H     | 1.69                     | 0.43              |
| 21:U:28:ARG:NH1   | 53:3:390:U:O2'     | 2.46                     | 0.43              |
| 27:b:153:LEU:HD23 | 51:1:1799:G:N2     | 2.33                     | 0.43              |
| 28:c:62:LYS:NZ    | 51:1:2810:A:H5''   | 2.34                     | 0.43              |
| 33:i:127:SER:OG   | 51:1:1059:G:N2     | 2.51                     | 0.43              |
| 37:m:96:ILE:HA    | 37:m:96:ILE:HD13   | 1.83                     | 0.43              |
| 38:n:39:PRO:HG2   | 51:1:1651:G:H4'    | 2.01                     | 0.43              |
| 51:1:68:G:H2'     | 51:1:69:C:O4'      | 2.18                     | 0.43              |
| 51:1:528:A:C2     | 51:1:2043:C:H4'    | 2.53                     | 0.43              |
| 51:1:1520:U:C2'   | 51:1:1521:G:H5'    | 2.49                     | 0.43              |
| 51:1:2106:U:H2'   | 51:1:2107:G:O4'    | 2.18                     | 0.43              |
| 51:1:2226:C:C5    | 51:1:2227:A:N7     | 2.86                     | 0.43              |
| 53:3:1513:A:H2'   | 53:3:1514:G:H8     | 1.83                     | 0.43              |
| 56:9:12:DC:H3'    | 58:B1:47:ARG:HH12  | 1.83                     | 0.43              |
| 1:A:62:LYS:HE3    | 1:A:62:LYS:HB3     | 1.89                     | 0.43              |
| 8:H:5:HIS:HE1     | 8:H:7:ASN:HB3      | 1.82                     | 0.43              |
| 8:H:76:ILE:HB     | 8:H:80:GLY:HA2     | 2.00                     | 0.43              |
| 10:J:28:ARG:NH2   | 53:3:1397:C:OP2    | 2.38                     | 0.43              |
| 10:J:146:MET:HE2  | 10:J:146:MET:HB3   | 1.75                     | 0.43              |
| 18:R:28:ARG:HH21  | 18:R:62:PHE:HB2    | 1.84                     | 0.43              |
| 23:W:33:THR:HG22  | 23:W:37:LYS:H      | 1.83                     | 0.43              |
| 27:b:48:ILE:HG12  | 51:1:779:U:OP2     | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:s:28:LYS:HE2    | 43:s:28:LYS:HB2    | 1.90                     | 0.43              |
| 43:s:74:ILE:HB     | 43:s:105:VAL:HG23  | 1.99                     | 0.43              |
| 45:u:76:THR:HB     | 45:u:78:LYS:HE3    | 1.99                     | 0.43              |
| 48:x:36:ARG:NH2    | 51:1:2200:C:OP2    | 2.52                     | 0.43              |
| 51:1:327:G:H2'     | 51:1:328:U:O4'     | 2.18                     | 0.43              |
| 51:1:473:G:C2'     | 51:1:474:G:H5'     | 2.48                     | 0.43              |
| 51:1:1433:A:H2'    | 51:1:1434:A:C1'    | 2.49                     | 0.43              |
| 51:1:1893:C:C2'    | 51:1:1894:C:H5'    | 2.47                     | 0.43              |
| 51:1:1998:A:O2'    | 51:1:1999:C:H5'    | 2.18                     | 0.43              |
| 51:1:2736:A:O2'    | 51:1:2737:G:H5'    | 2.19                     | 0.43              |
| 51:1:2870:C:H2'    | 51:1:2871:U:H5'    | 2.01                     | 0.43              |
| 53:3:422:C:H4'     | 53:3:423:G:C2      | 2.54                     | 0.43              |
| 53:3:490:C:H2'     | 53:3:491:G:H8      | 1.84                     | 0.43              |
| 53:3:560:A:H5''    | 53:3:561:U:H5'     | 2.00                     | 0.43              |
| 53:3:1200:C:O2'    | 53:3:1205:U:O4     | 2.35                     | 0.43              |
| 55:8:12:DG:OP1     | 58:B1:795:TYR:CE1  | 2.71                     | 0.43              |
| 57:A1:192:VAL:HG12 | 57:A1:193:GLU:H    | 1.83                     | 0.43              |
| 58:B1:62:PHE:CD1   | 58:B1:62:PHE:N     | 2.86                     | 0.43              |
| 58:B1:513:MET:HG3  | 58:B1:544:LEU:HD11 | 2.01                     | 0.43              |
| 65:0:545:ILE:HD11  | 65:0:581:GLY:HA3   | 2.00                     | 0.43              |
| 11:K:47:LEU:HG     | 11:K:56:LYS:HA     | 2.01                     | 0.43              |
| 24:X:27:LYS:HE2    | 24:X:27:LYS:HB3    | 1.77                     | 0.43              |
| 27:b:20:ASN:HB3    | 27:b:23:LEU:HD13   | 2.00                     | 0.43              |
| 29:d:127:GLU:O     | 29:d:156:ASN:ND2   | 2.51                     | 0.43              |
| 34:j:47:HIS:CG     | 51:1:536:G:N2      | 2.87                     | 0.43              |
| 34:j:47:HIS:CG     | 51:1:536:G:H21     | 2.37                     | 0.43              |
| 36:l:69:ARG:CZ     | 51:1:2406:A:N3     | 2.82                     | 0.43              |
| 37:m:69:PRO:HA     | 37:m:94:ALA:HB2    | 2.01                     | 0.43              |
| 38:n:103:ARG:HH11  | 51:1:1287:A:H5'    | 1.83                     | 0.43              |
| 51:1:255:A:H2'     | 51:1:256:A:O4'     | 2.18                     | 0.43              |
| 51:1:841:G:C2'     | 51:1:842:U:H5'     | 2.49                     | 0.43              |
| 51:1:1095:A:H3'    | 51:1:1096:A:H8     | 1.83                     | 0.43              |
| 51:1:1258:U:H2'    | 51:1:1259:G:C8     | 2.54                     | 0.43              |
| 51:1:1426:G:C6     | 51:1:1427:A:C6     | 3.06                     | 0.43              |
| 51:1:2305:U:O2'    | 51:1:2306:C:H5'    | 2.19                     | 0.43              |
| 51:1:2462:C:H2'    | 51:1:2463:C:C6     | 2.53                     | 0.43              |
| 57:A1:68:TYR:HE1   | 57:A1:79:LEU:HD13  | 1.83                     | 0.43              |
| 58:B1:59:ALA:HB1   | 58:B1:90:VAL:HG23  | 2.01                     | 0.43              |
| 58:B1:111:THR:CG2  | 58:B1:300:GLN:HA   | 2.48                     | 0.43              |
| 58:B1:434:ILE:HD11 | 59:B2:1274:GLU:HG3 | 2.00                     | 0.43              |
| 58:B1:515:ARG:HH12 | 58:B1:724:MET:HG2  | 1.84                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 58:B1:1024:THR:HG23 | 58:B1:1123:ARG:HA   | 2.00                     | 0.43              |
| 58:B1:1079:LYS:HD3  | 58:B1:1098:GLN:HB3  | 1.99                     | 0.43              |
| 58:B1:1108:GLN:HG3  | 58:B1:1109:LEU:HD12 | 1.99                     | 0.43              |
| 59:B2:590:PRO:HB2   | 59:B2:655:VAL:HG21  | 2.01                     | 0.43              |
| 31:f:84:LYS:HD2     | 31:f:84:LYS:HA      | 1.87                     | 0.43              |
| 37:m:17:ASN:OD1     | 37:m:97:GLN:NE2     | 2.51                     | 0.43              |
| 51:1:402:A:H2'      | 51:1:403:U:C5'      | 2.44                     | 0.43              |
| 51:1:623:C:O2'      | 51:1:624:C:H5'      | 2.18                     | 0.43              |
| 51:1:644:A:C3'      | 51:1:645:C:H5''     | 2.49                     | 0.43              |
| 51:1:993:G:O2'      | 51:1:994:C:H5'      | 2.19                     | 0.43              |
| 51:1:1092:C:H2'     | 51:1:1093:G:O4'     | 2.18                     | 0.43              |
| 51:1:1306:C:N4      | 51:1:1606:C:H2'     | 2.34                     | 0.43              |
| 51:1:1761:C:H2'     | 51:1:1762:A:O4'     | 2.18                     | 0.43              |
| 58:B1:107:LEU:HA    | 58:B1:276:ASN:ND2   | 2.33                     | 0.43              |
| 58:B1:220:ARG:NH1   | 58:B1:220:ARG:CG    | 2.82                     | 0.43              |
| 59:B2:11:ILE:HG22   | 59:B2:1172:LEU:HD11 | 1.99                     | 0.43              |
| 59:B2:22:LEU:HB3    | 59:B2:655:VAL:HG11  | 2.01                     | 0.43              |
| 59:B2:27:LEU:O      | 59:B2:528:ARG:NH1   | 2.43                     | 0.43              |
| 59:B2:300:ASP:OD1   | 59:B2:313:ALA:N     | 2.51                     | 0.43              |
| 59:B2:1157:GLN:HG3  | 59:B2:1159:VAL:HG13 | 2.00                     | 0.43              |
| 59:B2:1275:VAL:HG13 | 59:B2:1287:LEU:HD11 | 2.01                     | 0.43              |
| 7:G:107:ARG:HE      | 7:G:107:ARG:HB3     | 1.63                     | 0.43              |
| 8:H:106:ARG:HG2     | 8:H:107:LYS:HG3     | 2.01                     | 0.43              |
| 9:I:125:ASN:HB2     | 9:I:127:ARG:HD3     | 2.01                     | 0.43              |
| 13:M:24:VAL:HG23    | 13:M:60:LEU:HB2     | 2.00                     | 0.43              |
| 16:P:35:ASP:OD1     | 16:P:39:ASN:N       | 2.50                     | 0.43              |
| 17:Q:67:GLY:O       | 17:Q:98:ARG:NH1     | 2.52                     | 0.43              |
| 17:Q:113:ARG:NH1    | 53:3:36:C:O2'       | 2.51                     | 0.43              |
| 18:R:91:ARG:HD2     | 51:1:888:C:OP1      | 2.18                     | 0.43              |
| 27:b:206:LYS:HB2    | 51:1:729:G:C5       | 2.54                     | 0.43              |
| 41:q:83:LYS:HE2     | 41:q:83:LYS:HB3     | 1.72                     | 0.43              |
| 42:r:1:MET:HE3      | 42:r:101:ILE:HB     | 1.99                     | 0.43              |
| 44:t:40:LYS:HE3     | 44:t:60:THR:HG22    | 2.01                     | 0.43              |
| 49:y:11:VAL:HA      | 49:y:14:LEU:HB2     | 2.00                     | 0.43              |
| 51:1:131:A:H2'      | 51:1:132:G:C8       | 2.53                     | 0.43              |
| 51:1:705:A:C2       | 51:1:727:A:H1'      | 2.54                     | 0.43              |
| 51:1:783:A:C8       | 51:1:783:A:H3'      | 2.54                     | 0.43              |
| 51:1:871:U:H2'      | 51:1:872:U:C6       | 2.54                     | 0.43              |
| 51:1:1020:A:O5'     | 51:1:1020:A:H8      | 2.02                     | 0.43              |
| 51:1:1287:A:H3'     | 51:1:1288:G:N2      | 2.33                     | 0.43              |
| 51:1:1741:C:O2'     | 51:1:1742:U:H5'     | 2.18                     | 0.43              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 51:1:1751:U:H2'     | 51:1:1752:C:C6     | 2.54                     | 0.43              |
| 53:3:680:C:H2'      | 53:3:681:A:H8      | 1.84                     | 0.43              |
| 53:3:1209:C:O2'     | 53:3:1214:C:N4     | 2.52                     | 0.43              |
| 58:B1:45:ASN:HD22   | 58:B1:48:THR:H     | 1.65                     | 0.43              |
| 58:B1:102:MET:HG2   | 58:B1:246:PRO:CG   | 2.49                     | 0.43              |
| 59:B2:1313:HIS:CD2  | 60:W0:31:GLN:HE22  | 2.37                     | 0.43              |
| 65:0:438:LEU:HD13   | 65:0:469:ILE:HG23  | 2.01                     | 0.43              |
| 16:P:115:ILE:HD12   | 16:P:116:PRO:HD2   | 1.99                     | 0.43              |
| 24:X:6:LYS:NZ       | 53:3:1314:C:OP1    | 2.52                     | 0.43              |
| 27:b:7:PRO:HB3      | 27:b:13:ARG:HG3    | 1.99                     | 0.43              |
| 33:i:8:VAL:HG11     | 33:i:26:ALA:CB     | 2.49                     | 0.43              |
| 48:x:1:SER:OG       | 51:1:1365:A:OP2    | 2.35                     | 0.43              |
| 51:1:156:A:O2'      | 51:1:157:C:H5'     | 2.18                     | 0.43              |
| 51:1:467:G:O2'      | 51:1:468:G:H5'     | 2.19                     | 0.43              |
| 51:1:541:A:H2'      | 51:1:542:C:O4'     | 2.19                     | 0.43              |
| 51:1:758:C:H2'      | 51:1:759:G:H8      | 1.84                     | 0.43              |
| 51:1:864:G:C2'      | 51:1:865:C:H5'     | 2.48                     | 0.43              |
| 51:1:1172:C:H2'     | 51:1:1173:U:O4'    | 2.19                     | 0.43              |
| 51:1:1601:G:H2'     | 51:1:1602:U:H5'    | 2.01                     | 0.43              |
| 51:1:1917:U:H2'     | 51:1:1918:A:H5'    | 2.01                     | 0.43              |
| 51:1:1964:G:H4'     | 51:1:1965:C:OP2    | 2.19                     | 0.43              |
| 53:3:501:C:H2'      | 53:3:502:A:C8      | 2.53                     | 0.43              |
| 53:3:1348:U:H2'     | 53:3:1349:A:H8     | 1.84                     | 0.43              |
| 58:B1:388:ARG:HG2   | 58:B1:388:ARG:HH11 | 1.84                     | 0.43              |
| 58:B1:850:LYS:HB3   | 58:B1:855:ASP:HB2  | 2.00                     | 0.43              |
| 58:B1:1046:ILE:HG22 | 58:B1:1061:VAL:HA  | 2.00                     | 0.43              |
| 59:B2:546:GLU:H     | 59:B2:546:GLU:HG3  | 1.53                     | 0.43              |
| 63:5:9:A:H1'        | 63:5:45:U:H2'      | 2.01                     | 0.43              |
| 65:0:615:PRO:HB3    | 65:0:684:PHE:HE1   | 1.82                     | 0.43              |
| 7:G:122:ASP:N       | 7:G:122:ASP:OD1    | 2.51                     | 0.42              |
| 9:I:101:VAL:HG22    | 9:I:106:PHE:HB2    | 2.01                     | 0.42              |
| 31:f:151:ARG:HA     | 31:f:151:ARG:HD3   | 1.88                     | 0.42              |
| 36:l:108:ALA:HB3    | 36:l:125:LEU:HG    | 2.01                     | 0.42              |
| 51:1:918:A:H2'      | 51:1:919:U:O4'     | 2.19                     | 0.42              |
| 51:1:1536:C:H4'     | 51:1:1537:G:N1     | 2.32                     | 0.42              |
| 51:1:1668:A:C4'     | 51:1:1669:A:H5'    | 2.36                     | 0.42              |
| 51:1:2073:C:C2'     | 51:1:2074:U:H5'    | 2.49                     | 0.42              |
| 51:1:2371:G:O2'     | 51:1:2372:U:H5'    | 2.19                     | 0.42              |
| 51:1:2660:A:H2'     | 51:1:2661:G:O4'    | 2.18                     | 0.42              |
| 53:3:1005:A:OP2     | 53:3:1024:G:N2     | 2.48                     | 0.42              |
| 53:3:1442:G:H1      | 53:3:1460:C:H42    | 1.66                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:B1:824:PRO:HD3  | 58:B1:835:LEU:HD12 | 2.00                     | 0.42              |
| 59:B2:909:LYS:HD3  | 59:B2:909:LYS:HA   | 1.43                     | 0.42              |
| 65:0:557:ILE:CG2   | 65:0:576:ILE:HD12  | 2.48                     | 0.42              |
| 8:H:1:GLY:HA2      | 53:3:1060:U:C5     | 2.54                     | 0.42              |
| 10:J:110:MET:HA    | 10:J:113:VAL:HG12  | 2.01                     | 0.42              |
| 11:K:100:SER:O     | 11:K:100:SER:OG    | 2.34                     | 0.42              |
| 27:b:244:VAL:HG12  | 27:b:250:GLN:HA    | 2.01                     | 0.42              |
| 34:j:138:GLN:H     | 34:j:138:GLN:HG2   | 1.62                     | 0.42              |
| 40:p:63:ILE:HA     | 40:p:68:GLY:HA2    | 2.01                     | 0.42              |
| 47:w:14:ALA:HB1    | 51:1:2271:G:OP1    | 2.19                     | 0.42              |
| 51:1:8:C:C2        | 51:1:9:G:C8        | 3.07                     | 0.42              |
| 51:1:481:G:H2'     | 51:1:482:A:OP2     | 2.18                     | 0.42              |
| 51:1:712:G:C2'     | 51:1:713:G:H5'     | 2.49                     | 0.42              |
| 51:1:1487:U:H2'    | 51:1:1488:C:C6     | 2.54                     | 0.42              |
| 51:1:2844:G:H2'    | 51:1:2845:U:H6     | 1.80                     | 0.42              |
| 51:1:2895:G:H2'    | 51:1:2896:C:H6     | 1.84                     | 0.42              |
| 53:3:75:G:H1       | 53:3:95:C:H42      | 1.67                     | 0.42              |
| 58:B1:434:ILE:HD11 | 59:B2:1274:GLU:CG  | 2.49                     | 0.42              |
| 2:B:27:LEU:HD23    | 2:B:27:LEU:HA      | 1.84                     | 0.42              |
| 33:i:26:ALA:H      | 51:1:1070:A:H61    | 1.67                     | 0.42              |
| 33:i:129:GLU:HG3   | 33:i:139:VAL:HG21  | 2.00                     | 0.42              |
| 51:1:90:U:H2'      | 51:1:91:A:C8       | 2.55                     | 0.42              |
| 51:1:595:C:H2'     | 51:1:596:U:C6      | 2.54                     | 0.42              |
| 51:1:629:G:H2'     | 51:1:630:G:O4'     | 2.19                     | 0.42              |
| 51:1:673:C:O2'     | 51:1:674:G:H5'     | 2.19                     | 0.42              |
| 51:1:1020:A:H5'    | 51:1:1021:A:N7     | 2.34                     | 0.42              |
| 51:1:1087:G:H5''   | 51:1:1088:A:OP2    | 2.18                     | 0.42              |
| 51:1:1335:C:H2'    | 51:1:1336:A:H8     | 1.84                     | 0.42              |
| 51:1:1336:A:H2'    | 51:1:1337:G:H8     | 1.85                     | 0.42              |
| 51:1:1993:U:O2     | 51:1:1993:U:H2'    | 2.18                     | 0.42              |
| 51:1:2024:G:H2'    | 51:1:2025:C:C6     | 2.54                     | 0.42              |
| 51:1:2741:A:N6     | 51:1:2742:G:C2     | 2.88                     | 0.42              |
| 53:3:1253:G:H2'    | 53:3:1254:A:H8     | 1.83                     | 0.42              |
| 55:8:3:DC:N1       | 55:8:4:DT:H72      | 2.34                     | 0.42              |
| 58:B1:126:LEU:H    | 58:B1:126:LEU:HG   | 1.67                     | 0.42              |
| 58:B1:144:TYR:CE1  | 58:B1:162:GLU:OE1  | 2.73                     | 0.42              |
| 59:B2:125:GLY:H    | 59:B2:495:ALA:HB1  | 1.84                     | 0.42              |
| 12:L:68:VAL:HG23   | 12:L:99:ALA:HB1    | 2.02                     | 0.42              |
| 14:N:30:ASN:HD21   | 14:N:66:VAL:H      | 1.66                     | 0.42              |
| 14:N:98:ARG:HG2    | 14:N:103:VAL:HG21  | 2.00                     | 0.42              |
| 36:l:109:LYS:HE2   | 51:1:636:G:N7      | 2.34                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 41:q:54:ARG:HD3    | 51:1:1155:A:H5''    | 2.01                     | 0.42              |
| 43:s:87:PRO:HG3    | 51:1:1615:C:C6      | 2.54                     | 0.42              |
| 48:x:71:ARG:NH2    | 48:x:77:TYR:OH      | 2.42                     | 0.42              |
| 51:1:365:U:H2'     | 51:1:366:C:C6       | 2.53                     | 0.42              |
| 51:1:510:C:OP1     | 51:1:510:C:H3'      | 2.20                     | 0.42              |
| 51:1:535:G:O2'     | 51:1:536:G:H5'      | 2.20                     | 0.42              |
| 51:1:572:A:O5'     | 51:1:572:A:C8       | 2.72                     | 0.42              |
| 51:1:1306:C:H41    | 51:1:1606:C:H2'     | 1.84                     | 0.42              |
| 51:1:1500:G:H2'    | 51:1:1501:G:H8      | 1.83                     | 0.42              |
| 51:1:1907:G:C5     | 51:1:1908:C:C4      | 3.07                     | 0.42              |
| 51:1:1922:G:H4'    | 63:5:25:C:H4'       | 2.01                     | 0.42              |
| 51:1:2102:G:H1     | 51:1:2187:U:H3      | 1.66                     | 0.42              |
| 51:1:2287:A:C4     | 51:1:2289:G:N7      | 2.88                     | 0.42              |
| 51:1:2584:U:O5'    | 51:1:2584:U:H6      | 2.02                     | 0.42              |
| 53:3:460:A:H2'     | 53:3:461:A:C8       | 2.54                     | 0.42              |
| 55:8:15:DC:H5'     | 59:B2:1269:ARG:HD3  | 2.00                     | 0.42              |
| 57:A1:76:GLU:HB3   | 57:A1:80:GLU:HB3    | 2.01                     | 0.42              |
| 58:B1:58:CYS:SG    | 58:B1:60:ARG:HG2    | 2.59                     | 0.42              |
| 58:B1:96:LYS:NZ    | 59:B2:1298:VAL:HG11 | 2.34                     | 0.42              |
| 58:B1:111:THR:HG21 | 58:B1:303:VAL:HB    | 2.00                     | 0.42              |
| 58:B1:242:LEU:HA   | 58:B1:243:PRO:HD3   | 1.94                     | 0.42              |
| 58:B1:647:PRO:HG3  | 58:B1:697:MET:HB3   | 2.01                     | 0.42              |
| 58:B1:797:THR:HG22 | 58:B1:924:GLY:HA3   | 2.01                     | 0.42              |
| 59:B2:616:ILE:HG13 | 59:B2:652:TYR:HB2   | 2.01                     | 0.42              |
| 62:NG:130:PRO:HA   | 62:NG:148:VAL:O     | 2.20                     | 0.42              |
| 62:NG:135:ARG:O    | 62:NG:178:VAL:CA    | 2.68                     | 0.42              |
| 16:P:126:ARG:O     | 53:3:796:C:H5''     | 2.19                     | 0.42              |
| 17:Q:31:GLY:HA2    | 17:Q:56:LEU:HA      | 2.01                     | 0.42              |
| 24:X:36:ARG:HB3    | 53:3:1320:C:N4      | 2.34                     | 0.42              |
| 29:d:47:LYS:HE2    | 51:1:451:U:H4'      | 2.00                     | 0.42              |
| 39:o:33:ARG:O      | 39:o:65:THR:OG1     | 2.28                     | 0.42              |
| 48:x:55:MET:HE2    | 48:x:55:MET:HB3     | 1.91                     | 0.42              |
| 51:1:259:G:O2'     | 51:1:260:G:H5'      | 2.20                     | 0.42              |
| 51:1:1197:G:C2'    | 51:1:1198:U:H5'     | 2.50                     | 0.42              |
| 51:1:1230:A:H2'    | 51:1:1231:U:O4'     | 2.19                     | 0.42              |
| 51:1:2562:U:C2'    | 51:1:2563:U:H5'     | 2.49                     | 0.42              |
| 51:1:2839:G:O2'    | 51:1:2840:C:H5'     | 2.18                     | 0.42              |
| 51:1:2852:G:H2'    | 51:1:2853:C:O4'     | 2.20                     | 0.42              |
| 58:B1:244:VAL:HA   | 58:B1:269:TYR:OH    | 2.19                     | 0.42              |
| 58:B1:390:LEU:N    | 58:B1:390:LEU:HD13  | 2.35                     | 0.42              |
| 59:B2:11:ILE:O     | 59:B2:1149:TYR:OH   | 2.27                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:5:17:C:H6       | 63:5:17:C:H2'      | 1.69                     | 0.42              |
| 17:Q:50:LYS:HE2    | 17:Q:70:GLY:HA2    | 2.01                     | 0.42              |
| 20:T:66:LEU:HB3    | 20:T:77:TYR:HE1    | 1.84                     | 0.42              |
| 27:b:97:ASP:N      | 27:b:97:ASP:OD1    | 2.45                     | 0.42              |
| 29:d:53:THR:HB     | 51:1:452:G:H8      | 1.85                     | 0.42              |
| 32:g:11:ASN:ND2    | 51:1:2095:A:OP1    | 2.53                     | 0.42              |
| 39:o:40:ILE:HA     | 39:o:47:VAL:HA     | 2.00                     | 0.42              |
| 46:v:58:SER:OG     | 46:v:59:GLU:OE1    | 2.36                     | 0.42              |
| 51:1:623:C:H2'     | 51:1:624:C:H6      | 1.85                     | 0.42              |
| 51:1:648:G:H5''    | 51:1:2352:A:H5''   | 2.00                     | 0.42              |
| 51:1:870:U:H2'     | 51:1:871:U:C5'     | 2.48                     | 0.42              |
| 51:1:1054:A:H2'    | 51:1:1055:G:C8     | 2.54                     | 0.42              |
| 51:1:1316:U:O2'    | 51:1:1317:G:H5'    | 2.20                     | 0.42              |
| 51:1:1727:C:O2'    | 51:1:1728:C:H5'    | 2.20                     | 0.42              |
| 51:1:1886:U:O2'    | 51:1:1887:C:H5'    | 2.20                     | 0.42              |
| 51:1:2248:C:C2'    | 51:1:2249:U:H5'    | 2.49                     | 0.42              |
| 51:1:2292:U:H2'    | 51:1:2293:G:C8     | 2.55                     | 0.42              |
| 53:3:987:G:H2'     | 53:3:988:G:H8      | 1.84                     | 0.42              |
| 53:3:1531:A:C2'    | 53:3:1532:U:H5'    | 2.50                     | 0.42              |
| 58:B1:279:LEU:HD13 | 58:B1:299:LEU:HD13 | 2.02                     | 0.42              |
| 59:B2:557:ARG:HB3  | 59:B2:587:LEU:HD13 | 2.00                     | 0.42              |
| 2:B:39:ARG:HA      | 2:B:39:ARG:HD2     | 1.91                     | 0.42              |
| 9:I:55:ARG:HA      | 9:I:55:ARG:HD3     | 1.88                     | 0.42              |
| 13:M:52:GLY:HA3    | 13:M:56:PRO:HA     | 2.01                     | 0.42              |
| 17:Q:98:ARG:HA     | 17:Q:103:CYS:HB2   | 2.02                     | 0.42              |
| 18:R:11:HIS:HA     | 18:R:43:LYS:HD2    | 2.01                     | 0.42              |
| 18:R:87:GLY:O      | 18:R:91:ARG:N      | 2.52                     | 0.42              |
| 21:U:4:ILE:HG12    | 21:U:21:VAL:HG22   | 2.00                     | 0.42              |
| 42:r:62:GLU:HG3    | 42:r:97:LYS:HB3    | 2.01                     | 0.42              |
| 44:t:68:LYS:HD3    | 44:t:68:LYS:HA     | 1.83                     | 0.42              |
| 51:1:191:A:C2      | 51:1:192:C:C4      | 3.08                     | 0.42              |
| 51:1:532:A:H2'     | 51:1:532:A:N3      | 2.34                     | 0.42              |
| 51:1:849:A:H2'     | 51:1:850:U:C5      | 2.54                     | 0.42              |
| 51:1:955:U:H2'     | 51:1:956:G:H5'     | 2.02                     | 0.42              |
| 51:1:1204:A:H4'    | 51:1:1205:A:H5''   | 2.02                     | 0.42              |
| 51:1:1381:G:C2'    | 51:1:1382:G:H5'    | 2.49                     | 0.42              |
| 51:1:1642:G:H2'    | 51:1:1643:G:O4'    | 2.19                     | 0.42              |
| 51:1:1864:U:O5'    | 51:1:1864:U:H6     | 2.02                     | 0.42              |
| 51:1:2091:C:H5     | 51:1:2092:U:O2'    | 2.02                     | 0.42              |
| 51:1:2098:U:C2'    | 51:1:2099:U:H5'    | 2.49                     | 0.42              |
| 51:1:2144:G:H1'    | 51:1:2147:A:N6     | 2.34                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 58:B1:242:LEU:C    | 58:B1:242:LEU:HD23  | 2.44                     | 0.42              |
| 58:B1:243:PRO:HG2  | 59:B2:1332:SER:C    | 2.44                     | 0.42              |
| 58:B1:385:LEU:CD2  | 58:B1:390:LEU:HB2   | 2.50                     | 0.42              |
| 58:B1:568:SER:HB3  | 58:B1:570:LYS:NZ    | 2.34                     | 0.42              |
| 58:B1:616:PRO:HA   | 58:B1:619:ILE:HG22  | 2.02                     | 0.42              |
| 18:R:32:ILE:HG23   | 18:R:58:GLU:HB3     | 2.02                     | 0.42              |
| 18:R:89:ARG:HB2    | 18:R:96:VAL:HG22    | 2.01                     | 0.42              |
| 24:X:51:HIS:HB2    | 24:X:56:HIS:CE1     | 2.55                     | 0.42              |
| 28:c:175:LEU:HD12  | 28:c:175:LEU:HA     | 1.92                     | 0.42              |
| 33:i:78:LEU:HA     | 33:i:81:LYS:HB3     | 2.02                     | 0.42              |
| 38:n:16:HIS:CD2    | 51:1:1275:A:C2      | 3.07                     | 0.42              |
| 38:n:58:ASP:OD1    | 38:n:63:ARG:NH2     | 2.44                     | 0.42              |
| 51:1:128:C:H2'     | 51:1:129:C:C6       | 2.53                     | 0.42              |
| 51:1:439:A:H2'     | 51:1:440:C:O4'      | 2.19                     | 0.42              |
| 51:1:598:U:H2'     | 51:1:599:A:C8       | 2.54                     | 0.42              |
| 51:1:630:G:N2      | 51:1:634:C:C4       | 2.88                     | 0.42              |
| 51:1:809:G:C6      | 51:1:810:U:C4       | 3.08                     | 0.42              |
| 51:1:1936:A:N6     | 51:1:1963:U:H3      | 2.17                     | 0.42              |
| 51:1:2411:A:O2'    | 51:1:2412:A:H5'     | 2.20                     | 0.42              |
| 51:1:2697:G:C2     | 51:1:2711:A:C2      | 3.08                     | 0.42              |
| 53:3:322:C:O2      | 53:3:332:G:N2       | 2.52                     | 0.42              |
| 53:3:1513:A:H2'    | 53:3:1514:G:C8      | 2.55                     | 0.42              |
| 58:B1:362:ARG:HB2  | 58:B1:364:HIS:HD2   | 1.83                     | 0.42              |
| 58:B1:609:TYR:HD2  | 58:B1:610:ARG:NH1   | 2.17                     | 0.42              |
| 58:B1:839:VAL:HG12 | 58:B1:864:LEU:HD12  | 2.02                     | 0.42              |
| 58:B1:1350:ASN:HA  | 58:B1:1353:VAL:HG12 | 2.02                     | 0.42              |
| 59:B2:559:CYS:HA   | 59:B2:560:PRO:HD3   | 1.91                     | 0.42              |
| 59:B2:699:LEU:HG   | 59:B2:799:ASN:HD22  | 1.85                     | 0.42              |
| 59:B2:861:ALA:HB1  | 59:B2:882:ILE:HD13  | 2.01                     | 0.42              |
| 63:5:4:C:H2'       | 63:5:5:G:C8         | 2.55                     | 0.42              |
| 8:H:110:LEU:HD21   | 8:H:143:LEU:HB3     | 2.02                     | 0.42              |
| 9:I:24:VAL:HG22    | 53:3:409:U:H4'      | 2.02                     | 0.42              |
| 9:I:119:HIS:O      | 9:I:145:ARG:NH2     | 2.52                     | 0.42              |
| 14:N:84:ARG:NH2    | 53:3:1119:C:OP1     | 2.48                     | 0.42              |
| 14:N:113:LYS:HA    | 14:N:120:ALA:HB2    | 2.01                     | 0.42              |
| 27:b:57:HIS:ND1    | 51:1:1567:G:H5'     | 2.35                     | 0.42              |
| 28:c:134:HIS:HE1   | 51:1:1675:C:C4      | 2.38                     | 0.42              |
| 51:1:397:U:O5'     | 51:1:397:U:H6       | 2.02                     | 0.42              |
| 51:1:552:U:O2'     | 51:1:553:G:H5'      | 2.20                     | 0.42              |
| 51:1:1070:A:H5'    | 51:1:1072:C:OP1     | 2.20                     | 0.42              |
| 51:1:1467:U:C4     | 51:1:1468:U:C4      | 3.08                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1:1589:U:H2'    | 51:1:1590:A:C8     | 2.55                     | 0.42              |
| 51:1:1600:C:H2'    | 51:1:1601:G:C8     | 2.55                     | 0.42              |
| 51:1:1914:C:O2     | 51:1:1914:C:O4'    | 2.37                     | 0.42              |
| 51:1:2216:G:H2'    | 51:1:2217:G:C8     | 2.54                     | 0.42              |
| 51:1:2389:G:H5''   | 51:1:2390:U:H5'    | 2.01                     | 0.42              |
| 52:2:65:U:H3'      | 52:2:108:A:N6      | 2.30                     | 0.42              |
| 58:B1:141:PHE:CD2  | 58:B1:297:ARG:HB2  | 2.54                     | 0.42              |
| 58:B1:390:LEU:HD13 | 58:B1:390:LEU:H    | 1.85                     | 0.42              |
| 59:B2:741:MET:HE3  | 59:B2:974:ARG:HH12 | 1.85                     | 0.42              |
| 59:B2:829:THR:HG23 | 59:B2:1059:ARG:HG2 | 2.00                     | 0.42              |
| 8:H:61:LYS:HE2     | 8:H:96:VAL:HG12    | 2.01                     | 0.42              |
| 9:I:87:GLU:N       | 9:I:87:GLU:OE2     | 2.53                     | 0.42              |
| 10:J:90:GLY:O      | 10:J:129:SER:OG    | 2.36                     | 0.42              |
| 15:O:57:VAL:HG22   | 15:O:58:ASN:H      | 1.85                     | 0.42              |
| 38:n:28:LEU:O      | 38:n:32:GLU:N      | 2.38                     | 0.42              |
| 43:s:9:HIS:H       | 43:s:102:HIS:CE1   | 2.38                     | 0.42              |
| 51:1:4:U:O2'       | 51:1:5:A:H5'       | 2.20                     | 0.42              |
| 51:1:1181:U:H2'    | 51:1:1182:G:H8     | 1.81                     | 0.42              |
| 51:1:1213:A:C1'    | 51:1:1237:A:C2     | 3.03                     | 0.42              |
| 51:1:1314:C:H42    | 51:1:1338:G:H1     | 1.68                     | 0.42              |
| 51:1:1469:A:H2'    | 51:1:1470:A:H8     | 1.83                     | 0.42              |
| 51:1:1614:A:C8     | 51:1:1614:A:O5'    | 2.73                     | 0.42              |
| 53:3:73:C:H2'      | 53:3:74:A:C8       | 2.55                     | 0.42              |
| 53:3:842:U:H5''    | 53:3:846:G:C6      | 2.55                     | 0.42              |
| 58:B1:472:LEU:HD11 | 59:B2:1294:LYS:HG2 | 2.02                     | 0.42              |
| 58:B1:820:ILE:HD11 | 58:B1:822:MET:HE2  | 2.02                     | 0.42              |
| 58:B1:1289:ASN:O   | 58:B1:1293:GLU:HB2 | 2.20                     | 0.42              |
| 29:d:106:LYS:HG3   | 29:d:200:LEU:HD13  | 2.01                     | 0.41              |
| 29:d:145:ASP:HA    | 29:d:166:LYS:HB3   | 2.02                     | 0.41              |
| 50:z:57:GLU:OE1    | 50:z:57:GLU:N      | 2.53                     | 0.41              |
| 51:1:281:C:H2'     | 51:1:282:A:C8      | 2.54                     | 0.41              |
| 51:1:284:U:H2'     | 51:1:285:G:C8      | 2.55                     | 0.41              |
| 51:1:422:A:H2'     | 51:1:423:A:O4'     | 2.20                     | 0.41              |
| 51:1:837:C:O5'     | 51:1:837:C:H6      | 2.02                     | 0.41              |
| 51:1:1283:G:N2     | 51:1:1285:A:H3'    | 2.35                     | 0.41              |
| 51:1:1343:G:N3     | 51:1:1343:G:H2'    | 2.35                     | 0.41              |
| 51:1:1452:G:C2'    | 51:1:1453:A:OP2    | 2.68                     | 0.41              |
| 51:1:1719:G:O2'    | 51:1:1720:U:H5'    | 2.20                     | 0.41              |
| 51:1:1901:A:C2     | 51:1:1902:C:C5     | 3.08                     | 0.41              |
| 51:1:1983:G:HO2'   | 51:1:1984:G:H5'    | 1.82                     | 0.41              |
| 51:1:2583:G:H8     | 51:1:2583:G:O5'    | 2.03                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:1:2812:G:O2'   | 51:1:2813:A:H5'    | 2.19                     | 0.41              |
| 53:3:497:G:H2'    | 53:3:498:A:C8      | 2.55                     | 0.41              |
| 53:3:1243:C:H2'   | 53:3:1244:G:H8     | 1.84                     | 0.41              |
| 58:B1:175:GLU:H   | 58:B1:175:GLU:HG3  | 1.66                     | 0.41              |
| 58:B1:515:ARG:HG2 | 58:B1:516:ASP:H    | 1.85                     | 0.41              |
| 58:B1:950:ILE:HB  | 58:B1:1018:ALA:HB3 | 2.01                     | 0.41              |
| 63:5:27:G:H1      | 63:5:43:C:H42      | 1.68                     | 0.41              |
| 9:I:53:GLN:HA     | 9:I:198:LEU:HD12   | 2.01                     | 0.41              |
| 9:I:146:GLU:HA    | 9:I:149:LYS:HZ3    | 1.85                     | 0.41              |
| 23:W:24:ASP:OD1   | 23:W:24:ASP:N      | 2.53                     | 0.41              |
| 26:Z:39:LYS:HA    | 26:Z:42:THR:HB     | 2.02                     | 0.41              |
| 27:b:109:LEU:HD12 | 27:b:109:LEU:HA    | 1.93                     | 0.41              |
| 44:t:28:ASN:HD21  | 44:t:91:GLN:HB3    | 1.85                     | 0.41              |
| 45:u:6:ARG:N      | 51:1:85:G:OP1      | 2.52                     | 0.41              |
| 51:1:638:G:H2'    | 51:1:639:U:C6      | 2.55                     | 0.41              |
| 51:1:724:U:C4     | 51:1:725:G:C6      | 3.08                     | 0.41              |
| 51:1:1034:G:C6    | 51:1:1035:U:N3     | 2.88                     | 0.41              |
| 51:1:1048:A:C2'   | 51:1:1049:C:H5'    | 2.49                     | 0.41              |
| 51:1:1077:A:H3'   | 51:1:1078:U:H4'    | 2.02                     | 0.41              |
| 51:1:1482:G:H2'   | 51:1:1483:G:H8     | 1.85                     | 0.41              |
| 51:1:1594:U:O2'   | 51:1:1595:C:H5'    | 2.20                     | 0.41              |
| 51:1:1812:U:H5''  | 51:1:1812:U:H6     | 1.85                     | 0.41              |
| 51:1:2160:C:H2'   | 51:1:2161:C:O4'    | 2.20                     | 0.41              |
| 51:1:2437:G:O4'   | 51:1:2598:A:C2     | 2.73                     | 0.41              |
| 51:1:2467:C:N4    | 51:1:2468:A:C6     | 2.89                     | 0.41              |
| 51:1:2612:C:O5'   | 51:1:2612:C:H6     | 2.03                     | 0.41              |
| 58:B1:137:ARG:HA  | 58:B1:142:GLU:HG2  | 2.02                     | 0.41              |
| 58:B1:144:TYR:CD1 | 58:B1:144:TYR:N    | 2.88                     | 0.41              |
| 59:B2:22:LEU:HD22 | 59:B2:603:ILE:HG21 | 2.02                     | 0.41              |
| 7:G:17:HIS:C      | 7:G:19:THR:H       | 2.28                     | 0.41              |
| 28:c:136:ASN:ND2  | 28:c:139:SER:O     | 2.52                     | 0.41              |
| 33:i:116:MET:HE2  | 33:i:116:MET:HB3   | 1.79                     | 0.41              |
| 34:j:109:LEU:HD23 | 34:j:109:LEU:HA    | 1.85                     | 0.41              |
| 51:1:49:A:P       | 51:1:51:G:H5'      | 2.61                     | 0.41              |
| 51:1:196:A:N3     | 51:1:196:A:H2'     | 2.35                     | 0.41              |
| 51:1:256:A:C2'    | 51:1:257:C:H5'     | 2.50                     | 0.41              |
| 51:1:759:G:H2'    | 51:1:760:G:H8      | 1.83                     | 0.41              |
| 51:1:1152:C:H2'   | 51:1:1153:C:C6     | 2.55                     | 0.41              |
| 51:1:1246:A:H2'   | 51:1:1247:A:O4'    | 2.19                     | 0.41              |
| 51:1:1822:C:H2'   | 51:1:1823:G:H8     | 1.85                     | 0.41              |
| 51:1:1991:U:H2'   | 51:1:1992:G:H5'    | 2.02                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:1:2628:C:H3'    | 51:1:2629:U:H5'   | 2.01                     | 0.41              |
| 53:3:1238:A:OP1    | 53:3:1335:U:O2'   | 2.35                     | 0.41              |
| 53:3:1382:C:H2'    | 53:3:1383:C:H6    | 1.84                     | 0.41              |
| 58:B1:576:ARG:HD3  | 58:B1:593:ASN:HA  | 2.02                     | 0.41              |
| 59:B2:50:GLU:HG2   | 59:B2:73:TYR:HE1  | 1.85                     | 0.41              |
| 59:B2:478:ARG:HD2  | 59:B2:492:MET:HA  | 2.02                     | 0.41              |
| 59:B2:1244:HIS:NE2 | 59:B2:1266:GLY:O  | 2.44                     | 0.41              |
| 63:5:29:G:H2'      | 63:5:29:G:N3      | 2.35                     | 0.41              |
| 7:G:162:VAL:N      | 7:G:183:PHE:O     | 2.38                     | 0.41              |
| 11:K:40:GLU:HB3    | 11:K:61:LEU:HB3   | 2.02                     | 0.41              |
| 13:M:26:MET:HE2    | 13:M:26:MET:HB3   | 1.96                     | 0.41              |
| 28:c:4:LEU:HD21    | 28:c:98:VAL:HA    | 2.02                     | 0.41              |
| 35:k:7:MET:HE2     | 35:k:18:ARG:HD3   | 2.01                     | 0.41              |
| 40:p:110:LYS:HE3   | 40:p:110:LYS:HB3  | 1.91                     | 0.41              |
| 41:q:23:TYR:HB3    | 41:q:27:ARG:HB2   | 2.02                     | 0.41              |
| 46:v:14:LYS:HB2    | 52:2:98:G:H1      | 1.84                     | 0.41              |
| 47:w:7:ARG:HA      | 47:w:7:ARG:HD3    | 1.77                     | 0.41              |
| 51:1:573:U:O2'     | 51:1:574:A:H3'    | 2.20                     | 0.41              |
| 51:1:1038:G:H2'    | 51:1:1039:A:H8    | 1.83                     | 0.41              |
| 51:1:1173:U:H5     | 51:1:1174:U:H1'   | 1.81                     | 0.41              |
| 51:1:1239:G:H2'    | 51:1:1240:U:O4'   | 2.21                     | 0.41              |
| 51:1:1418:G:H1'    | 51:1:1581:G:N2    | 2.36                     | 0.41              |
| 51:1:1750:G:H2'    | 51:1:1751:U:C6    | 2.56                     | 0.41              |
| 51:1:2156:G:H2'    | 51:1:2157:G:C5'   | 2.35                     | 0.41              |
| 51:1:2741:A:H2'    | 51:1:2742:G:C5'   | 2.50                     | 0.41              |
| 53:3:142:G:O2'     | 53:3:196:A:N1     | 2.45                     | 0.41              |
| 55:8:14:DC:C2      | 55:8:15:DC:C5     | 3.09                     | 0.41              |
| 57:A2:104:LYS:O    | 57:A2:139:SER:OG  | 2.36                     | 0.41              |
| 58:B1:239:LEU:HD23 | 58:B1:239:LEU:N   | 2.36                     | 0.41              |
| 58:B1:395:LYS:HB3  | 58:B1:395:LYS:HE3 | 1.45                     | 0.41              |
| 59:B2:515:MET:HE2  | 59:B2:515:MET:HB3 | 1.82                     | 0.41              |
| 65:0:491:ARG:HD3   | 65:0:491:ARG:HA   | 1.71                     | 0.41              |
| 1:A:2:LYS:NZ       | 52:2:42:C:OP2     | 2.39                     | 0.41              |
| 31:f:21:GLN:NE2    | 31:f:37:ASN:O     | 2.54                     | 0.41              |
| 31:f:81:GLY:HA3    | 31:f:133:LYS:HZ1  | 1.85                     | 0.41              |
| 51:1:191:A:H2'     | 51:1:192:C:C6     | 2.56                     | 0.41              |
| 51:1:903:C:H2'     | 51:1:904:G:H8     | 1.86                     | 0.41              |
| 51:1:1063:G:N2     | 51:1:1075:C:H41   | 2.18                     | 0.41              |
| 51:1:1553:A:O2'    | 51:1:1554:U:H5    | 2.02                     | 0.41              |
| 51:1:1599:U:H2'    | 51:1:1600:C:H6    | 1.85                     | 0.41              |
| 51:1:1868:C:H2'    | 51:1:1869:G:H8    | 1.86                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 51:1:2482:A:H2'     | 51:1:2483:C:C6      | 2.54                     | 0.41              |
| 53:3:370:C:H2'      | 53:3:371:A:H8       | 1.86                     | 0.41              |
| 53:3:373:A:N1       | 53:3:391:G:O2'      | 2.49                     | 0.41              |
| 53:3:1228:C:H2'     | 53:3:1229:A:C8      | 2.55                     | 0.41              |
| 57:A1:48:LEU:HD12   | 57:A1:48:LEU:HA     | 1.79                     | 0.41              |
| 58:B1:1050:THR:HG23 | 58:B1:1057:SER:HB3  | 2.03                     | 0.41              |
| 58:B1:1177:ILE:HD12 | 58:B1:1186:TYR:HE2  | 1.85                     | 0.41              |
| 58:B1:1223:LEU:HA   | 58:B1:1223:LEU:HD23 | 1.89                     | 0.41              |
| 59:B2:979:LEU:HD11  | 59:B2:1011:LEU:HD11 | 2.03                     | 0.41              |
| 59:B2:1278:LEU:HA   | 59:B2:1278:LEU:HD23 | 1.86                     | 0.41              |
| 27:b:107:LYS:HE2    | 27:b:107:LYS:HB2    | 1.87                     | 0.41              |
| 35:k:17:ARG:HD3     | 35:k:47:ILE:HD11    | 2.02                     | 0.41              |
| 50:z:31:ILE:HD11    | 51:1:989:G:P        | 2.61                     | 0.41              |
| 51:1:115:C:O2'      | 51:1:116:C:H5'      | 2.20                     | 0.41              |
| 51:1:127:A:H5''     | 51:1:128:C:O4'      | 2.21                     | 0.41              |
| 51:1:431:U:O5'      | 51:1:431:U:H6       | 2.03                     | 0.41              |
| 51:1:688:U:O5'      | 51:1:688:U:H6       | 2.03                     | 0.41              |
| 51:1:877:A:H2'      | 51:1:878:A:H5''     | 2.02                     | 0.41              |
| 51:1:892:A:O2'      | 51:1:893:C:H5'      | 2.19                     | 0.41              |
| 51:1:940:G:H2'      | 51:1:941:A:C4'      | 2.51                     | 0.41              |
| 51:1:1045:C:H1'     | 51:1:1047:G:C2      | 2.56                     | 0.41              |
| 51:1:1488:C:H2'     | 51:1:1489:C:H6      | 1.84                     | 0.41              |
| 53:3:202:G:H2'      | 53:3:203:G:C8       | 2.55                     | 0.41              |
| 53:3:685:G:N1       | 53:3:704:A:OP2      | 2.52                     | 0.41              |
| 58:B1:24:LEU:HD21   | 58:B1:116:PHE:CE2   | 2.54                     | 0.41              |
| 58:B1:71:LEU:HD23   | 58:B1:71:LEU:HA     | 1.75                     | 0.41              |
| 58:B1:224:LEU:HD23  | 58:B1:224:LEU:HA    | 1.89                     | 0.41              |
| 58:B1:559:ALA:HB3   | 58:B1:562:GLU:HB3   | 2.01                     | 0.41              |
| 58:B1:820:ILE:HG12  | 58:B1:884:SER:HB2   | 2.01                     | 0.41              |
| 59:B2:469:VAL:HA    | 59:B2:472:GLU:HG2   | 2.02                     | 0.41              |
| 59:B2:755:LYS:HD2   | 59:B2:755:LYS:HA    | 1.86                     | 0.41              |
| 65:0:298:ILE:CG2    | 65:0:304:ASP:HA     | 2.50                     | 0.41              |
| 8:H:178:ARG:NH1     | 53:3:1112:C:O2'     | 2.54                     | 0.41              |
| 9:I:44:LYS:HA       | 9:I:44:LYS:HD2      | 1.55                     | 0.41              |
| 16:P:30:ILE:HG23    | 16:P:45:THR:HB      | 2.02                     | 0.41              |
| 28:c:59:ARG:HD3     | 28:c:59:ARG:HA      | 1.83                     | 0.41              |
| 28:c:90:PHE:HD1     | 28:c:94:GLN:HG2     | 1.83                     | 0.41              |
| 37:m:123:LYS:HE2    | 51:1:2467:C:O2      | 2.20                     | 0.41              |
| 51:1:94:A:H2'       | 51:1:95:A:C8        | 2.54                     | 0.41              |
| 51:1:244:A:H2'      | 51:1:245:G:O4'      | 2.20                     | 0.41              |
| 51:1:426:C:O2'      | 51:1:427:U:H5'      | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1:543:G:C3'     | 51:1:544:C:H5''    | 2.51                     | 0.41              |
| 51:1:1024:G:H21    | 51:1:1144:A:C4'    | 2.33                     | 0.41              |
| 51:1:1416:G:H2'    | 51:1:1417:C:H6     | 1.82                     | 0.41              |
| 51:1:2335:A:N7     | 51:1:2337:G:C5     | 2.88                     | 0.41              |
| 51:1:2568:U:O5'    | 51:1:2568:U:H6     | 2.04                     | 0.41              |
| 51:1:2743:U:H2'    | 51:1:2744:G:C4'    | 2.50                     | 0.41              |
| 53:3:146:G:H2'     | 53:3:147:G:C8      | 2.56                     | 0.41              |
| 57:A1:33:ARG:HE    | 57:A1:33:ARG:HB3   | 1.56                     | 0.41              |
| 58:B1:848:VAL:HB   | 58:B1:858:VAL:HG22 | 2.02                     | 0.41              |
| 59:B2:524:ILE:HD12 | 59:B2:712:SER:HB2  | 2.02                     | 0.41              |
| 59:B2:646:SER:OG   | 59:B2:647:ARG:N    | 2.51                     | 0.41              |
| 59:B2:870:ILE:HB   | 59:B2:944:ARG:HD3  | 2.02                     | 0.41              |
| 59:B2:998:LEU:HD21 | 59:B2:1015:ALA:HB2 | 2.02                     | 0.41              |
| 65:0:519:VAL:HB    | 65:0:580:PHE:HB3   | 2.02                     | 0.41              |
| 6:F:35:GLN:HE21    | 6:F:35:GLN:HB3     | 1.57                     | 0.41              |
| 12:L:125:ASP:HB2   | 12:L:130:LYS:HG3   | 2.03                     | 0.41              |
| 25:Y:4:LYS:HA      | 25:Y:4:LYS:HD3     | 1.86                     | 0.41              |
| 51:1:170:U:H2'     | 51:1:171:U:C6      | 2.55                     | 0.41              |
| 51:1:197:A:H2      | 51:1:2434:A:H62    | 1.69                     | 0.41              |
| 51:1:265:A:C8      | 51:1:428:A:C2      | 3.09                     | 0.41              |
| 51:1:490:C:O2'     | 51:1:491:G:P       | 2.79                     | 0.41              |
| 51:1:908:C:O2'     | 51:1:909:A:H5'     | 2.19                     | 0.41              |
| 51:1:1317:G:H2'    | 51:1:1318:U:C6     | 2.56                     | 0.41              |
| 51:1:1327:A:H2'    | 51:1:1328:A:H5'    | 2.01                     | 0.41              |
| 51:1:1782:U:C2'    | 51:1:1783:A:H5''   | 2.51                     | 0.41              |
| 51:1:1931:U:C5     | 51:1:1968:G:N2     | 2.88                     | 0.41              |
| 51:1:1955:U:H5     | 51:1:2557:G:N2     | 2.19                     | 0.41              |
| 51:1:2098:U:H2'    | 51:1:2099:U:H5'    | 2.03                     | 0.41              |
| 51:1:2615:U:O2     | 51:1:2615:U:H2'    | 2.20                     | 0.41              |
| 51:1:2848:G:C2     | 51:1:2867:G:C4     | 3.08                     | 0.41              |
| 58:B1:109:SER:HA   | 58:B1:110:PRO:HD3  | 1.96                     | 0.41              |
| 58:B1:450:HIS:HA   | 58:B1:451:PRO:HD3  | 1.91                     | 0.41              |
| 58:B1:586:GLY:HA3  | 58:B1:612:LEU:HD11 | 2.01                     | 0.41              |
| 59:B2:310:ILE:HG21 | 59:B2:325:LEU:HB3  | 2.03                     | 0.41              |
| 59:B2:678:ARG:HD3  | 59:B2:678:ARG:HA   | 1.84                     | 0.41              |
| 59:B2:741:MET:SD   | 59:B2:974:ARG:NH2  | 2.93                     | 0.41              |
| 5:E:28:LEU:HD23    | 5:E:28:LEU:HA      | 1.83                     | 0.41              |
| 8:H:19:SER:HB2     | 8:H:39:ARG:HH21    | 1.85                     | 0.41              |
| 15:O:12:ALA:HB2    | 15:O:96:VAL:HG13   | 2.03                     | 0.41              |
| 16:P:17:ASP:OD1    | 16:P:17:ASP:N      | 2.44                     | 0.41              |
| 18:R:10:ASP:HB3    | 18:R:45:SER:HB3    | 2.03                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:U:63:GLN:OE1    | 53:3:227:G:O2'     | 2.36                     | 0.41              |
| 21:U:68:SER:OG     | 21:U:69:ASP:N      | 2.53                     | 0.41              |
| 30:e:39:VAL:HG12   | 30:e:85:GLY:HA2    | 2.03                     | 0.41              |
| 31:f:60:GLY:O      | 31:f:64:ALA:N      | 2.53                     | 0.41              |
| 33:i:41:PHE:O      | 33:i:45:THR:N      | 2.54                     | 0.41              |
| 33:i:77:VAL:HA     | 33:i:80:LYS:HE2    | 2.02                     | 0.41              |
| 33:i:89:SER:HB3    | 51:1:1063:G:O2'    | 2.20                     | 0.41              |
| 33:i:109:ALA:O     | 33:i:113:ALA:N     | 2.53                     | 0.41              |
| 42:r:81:LYS:NZ     | 51:1:568:U:O4      | 2.54                     | 0.41              |
| 43:s:29:VAL:HG21   | 43:s:55:ILE:HG21   | 2.03                     | 0.41              |
| 51:1:56:A:H1'      | 51:1:127:A:C2      | 2.55                     | 0.41              |
| 51:1:79:C:O2       | 51:1:346:A:H2      | 2.03                     | 0.41              |
| 51:1:191:A:C6      | 51:1:192:C:N4      | 2.88                     | 0.41              |
| 51:1:235:U:H2'     | 51:1:236:C:H6      | 1.86                     | 0.41              |
| 51:1:309:A:N3      | 51:1:329:G:O2'     | 2.53                     | 0.41              |
| 51:1:518:G:H2'     | 51:1:519:U:C6      | 2.55                     | 0.41              |
| 51:1:679:C:H2'     | 51:1:680:C:C6      | 2.56                     | 0.41              |
| 51:1:924:G:O2'     | 51:1:925:A:H5'     | 2.21                     | 0.41              |
| 51:1:1095:A:C1'    | 65:0:632:ILE:HD13  | 2.51                     | 0.41              |
| 51:1:1107:G:H2'    | 51:1:1108:U:C6     | 2.56                     | 0.41              |
| 51:1:1107:G:H2'    | 51:1:1108:U:O4'    | 2.20                     | 0.41              |
| 51:1:1328:A:H2'    | 51:1:1330:C:C4     | 2.56                     | 0.41              |
| 51:1:2575:C:H2'    | 51:1:2578:G:O6     | 2.21                     | 0.41              |
| 51:1:2600:A:H8     | 51:1:2600:A:O5'    | 2.03                     | 0.41              |
| 51:1:2660:A:H2'    | 51:1:2661:G:C8     | 2.56                     | 0.41              |
| 53:3:146:G:H2'     | 53:3:147:G:H8      | 1.86                     | 0.41              |
| 53:3:1304:G:N1     | 53:3:1332:A:OP2    | 2.54                     | 0.41              |
| 58:B1:108:ALA:HB2  | 58:B1:276:ASN:OD1  | 2.21                     | 0.41              |
| 58:B1:109:SER:CB   | 58:B1:296:LYS:HG2  | 2.51                     | 0.41              |
| 58:B1:111:THR:HG23 | 58:B1:300:GLN:HA   | 2.03                     | 0.41              |
| 58:B1:1272:SER:OG  | 58:B1:1273:ASP:N   | 2.53                     | 0.41              |
| 59:B2:176:ILE:HD12 | 59:B2:184:LEU:HD23 | 2.03                     | 0.41              |
| 59:B2:213:LEU:HD13 | 59:B2:422:LYS:HG2  | 2.03                     | 0.41              |
| 62:NG:175:PHE:O    | 62:NG:178:VAL:O    | 2.38                     | 0.41              |
| 8:H:14:VAL:HG11    | 8:H:180:ASP:HB3    | 2.03                     | 0.41              |
| 32:g:1:MET:N       | 32:g:20:ASN:OD1    | 2.40                     | 0.41              |
| 38:n:22:ARG:HH22   | 51:1:2709:G:H5'    | 1.86                     | 0.41              |
| 38:n:71:ARG:HE     | 38:n:71:ARG:HB3    | 1.68                     | 0.41              |
| 39:o:24:THR:HB     | 39:o:42:PRO:HG3    | 2.02                     | 0.41              |
| 51:1:10:A:C6       | 51:1:2800:A:C2     | 3.09                     | 0.41              |
| 51:1:224:U:O4      | 51:1:420:C:H5'     | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:1:518:G:C2     | 51:1:519:U:C2     | 3.08                     | 0.41              |
| 51:1:722:A:H2'    | 51:1:723:C:C6     | 2.56                     | 0.41              |
| 51:1:1116:G:O2'   | 51:1:1117:C:H5'   | 2.22                     | 0.41              |
| 51:1:1412:U:H2'   | 51:1:1413:A:C8    | 2.56                     | 0.41              |
| 51:1:1605:C:H2'   | 51:1:1606:C:C5'   | 2.51                     | 0.41              |
| 51:1:2649:C:N3    | 51:1:2650:U:C4    | 2.89                     | 0.41              |
| 51:1:2701:U:H3'   | 51:1:2702:G:H5''  | 2.01                     | 0.41              |
| 51:1:2776:A:C6    | 51:1:2778:A:C6    | 3.09                     | 0.41              |
| 53:3:336:A:H2'    | 53:3:337:G:H8     | 1.86                     | 0.41              |
| 58:B1:68:TYR:CB   | 58:B1:75:TYR:HE2  | 2.34                     | 0.41              |
| 58:B1:245:LEU:HG  | 58:B1:246:PRO:CD  | 2.50                     | 0.41              |
| 7:G:190:SER:OG    | 7:G:191:ASP:N     | 2.53                     | 0.40              |
| 9:I:101:VAL:HG13  | 9:I:113:ALA:HB1   | 2.03                     | 0.40              |
| 13:M:42:GLU:HG2   | 13:M:100:ILE:HG21 | 2.02                     | 0.40              |
| 16:P:108:ASN:HA   | 26:Z:7:GLU:HG2    | 2.03                     | 0.40              |
| 24:X:49:ALA:HA    | 24:X:58:PRO:HA    | 2.03                     | 0.40              |
| 28:c:169:ARG:O    | 51:1:2773:C:H4'   | 2.21                     | 0.40              |
| 29:d:163:ASN:HD21 | 51:1:322:A:P      | 2.45                     | 0.40              |
| 30:e:124:ARG:NH2  | 51:1:2315:G:N3    | 2.68                     | 0.40              |
| 35:k:44:LYS:HB3   | 35:k:44:LYS:HE3   | 1.92                     | 0.40              |
| 42:r:4:VAL:HG23   | 42:r:39:LEU:HB2   | 2.03                     | 0.40              |
| 51:1:724:U:H2'    | 51:1:725:G:O4'    | 2.21                     | 0.40              |
| 51:1:1092:C:O2'   | 51:1:1093:G:H5'   | 2.21                     | 0.40              |
| 51:1:1302:A:H5'   | 51:1:1608:A:OP1   | 2.21                     | 0.40              |
| 51:1:1722:A:H2'   | 51:1:1723:G:O4'   | 2.21                     | 0.40              |
| 51:1:2221:G:H2'   | 51:1:2222:C:C6    | 2.56                     | 0.40              |
| 51:1:2293:G:O2'   | 51:1:2294:G:H5'   | 2.21                     | 0.40              |
| 51:1:2379:G:H2'   | 51:1:2380:C:C6    | 2.56                     | 0.40              |
| 51:1:2828:G:N1    | 51:1:2829:A:C5    | 2.90                     | 0.40              |
| 58:B1:144:TYR:OH  | 58:B1:162:GLU:OE1 | 2.34                     | 0.40              |
| 63:5:17:C:H2'     | 63:5:18:G:C8      | 2.56                     | 0.40              |
| 65:0:118:GLY:HA2  | 65:0:154:VAL:HG22 | 2.03                     | 0.40              |
| 7:G:104:LYS:HE2   | 7:G:104:LYS:HB2   | 1.92                     | 0.40              |
| 9:I:10:LEU:HG     | 9:I:62:ARG:HD2    | 2.03                     | 0.40              |
| 13:M:91:LEU:HD23  | 13:M:91:LEU:HA    | 1.90                     | 0.40              |
| 14:N:22:PRO:HA    | 14:N:60:LEU:HA    | 2.03                     | 0.40              |
| 15:O:89:ARG:NH2   | 62:NG:165:PHE:H   | 2.18                     | 0.40              |
| 20:T:80:LEU:HD12  | 20:T:80:LEU:HA    | 1.91                     | 0.40              |
| 22:V:7:LEU:N      | 22:V:59:GLU:OE2   | 2.53                     | 0.40              |
| 22:V:52:CYS:HB3   | 22:V:58:VAL:HG11  | 2.03                     | 0.40              |
| 25:Y:43:LYS:HE2   | 25:Y:43:LYS:HB2   | 1.88                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1:211:C:O2'     | 51:1:212:G:H5'     | 2.21                     | 0.40              |
| 51:1:379:G:N1      | 51:1:396:G:C6      | 2.89                     | 0.40              |
| 51:1:555:G:HO2'    | 51:1:556:A:H8      | 1.69                     | 0.40              |
| 51:1:1048:A:N6     | 51:1:1111:A:C8     | 2.89                     | 0.40              |
| 51:1:1430:G:O2'    | 51:1:1431:A:H5'    | 2.21                     | 0.40              |
| 51:1:1715:G:O2'    | 51:1:1716:U:C6     | 2.75                     | 0.40              |
| 51:1:1721:G:H1'    | 51:1:1739:A:N6     | 2.35                     | 0.40              |
| 51:1:2648:G:O2'    | 51:1:2649:C:H5'    | 2.21                     | 0.40              |
| 51:1:2680:U:O2'    | 51:1:2681:C:H5'    | 2.21                     | 0.40              |
| 53:3:31:G:N2       | 53:3:48:C:OP1      | 2.41                     | 0.40              |
| 58:B1:26:SER:HB3   | 58:B1:29:MET:H     | 1.86                     | 0.40              |
| 58:B1:282:LEU:CA   | 58:B1:286:ALA:HA   | 2.45                     | 0.40              |
| 59:B2:657:THR:HG21 | 59:B2:1188:ASP:HB2 | 2.03                     | 0.40              |
| 59:B2:886:LYS:HE2  | 59:B2:918:LEU:HD13 | 2.03                     | 0.40              |
| 63:5:23:A:H2'      | 63:5:24:G:C8       | 2.56                     | 0.40              |
| 6:F:30:GLU:HA      | 6:F:31:PRO:HD3     | 1.91                     | 0.40              |
| 7:G:130:LYS:HE3    | 7:G:130:LYS:HB3    | 1.96                     | 0.40              |
| 8:H:5:HIS:HA       | 8:H:6:PRO:HD3      | 1.95                     | 0.40              |
| 18:R:7:ASN:CG      | 18:R:9:PRO:HD2     | 2.45                     | 0.40              |
| 18:R:41:ASP:OD1    | 18:R:41:ASP:N      | 2.54                     | 0.40              |
| 27:b:70:LYS:HD2    | 27:b:73:ILE:HD12   | 2.02                     | 0.40              |
| 30:e:64:PRO:HA     | 30:e:88:VAL:HG22   | 2.03                     | 0.40              |
| 31:f:3:VAL:HG13    | 51:1:2751:G:H4'    | 2.02                     | 0.40              |
| 35:k:13:ASN:HB3    | 35:k:100:PHE:CZ    | 2.57                     | 0.40              |
| 35:k:110:GLU:H     | 35:k:113:MET:HE3   | 1.86                     | 0.40              |
| 45:u:4:ILE:HD13    | 45:u:69:VAL:HG23   | 2.03                     | 0.40              |
| 51:1:137:U:H3      | 51:1:142:A:H61     | 1.69                     | 0.40              |
| 51:1:467:G:O5'     | 51:1:467:G:H8      | 2.04                     | 0.40              |
| 51:1:886:A:N7      | 51:1:887:U:H1'     | 2.36                     | 0.40              |
| 51:1:1095:A:H1'    | 65:0:632:ILE:HD13  | 2.02                     | 0.40              |
| 51:1:1333:G:C2'    | 51:1:1334:G:H5'    | 2.51                     | 0.40              |
| 51:1:1346:G:O2'    | 51:1:1347:A:H5'    | 2.22                     | 0.40              |
| 51:1:1505:A:O2'    | 51:1:1506:U:H5'    | 2.19                     | 0.40              |
| 51:1:1767:G:N2     | 51:1:1986:C:C2     | 2.89                     | 0.40              |
| 51:1:2049:G:O2'    | 51:1:2050:C:H5'    | 2.21                     | 0.40              |
| 51:1:2105:U:C2     | 51:1:2184:A:H2     | 2.39                     | 0.40              |
| 51:1:2106:U:H3'    | 51:1:2107:G:H8     | 1.86                     | 0.40              |
| 51:1:2193:G:H2'    | 51:1:2194:U:H6     | 1.83                     | 0.40              |
| 51:1:2210:U:H6     | 51:1:2210:U:OP1    | 2.04                     | 0.40              |
| 51:1:2357:G:C2     | 51:1:2361:G:C6     | 3.09                     | 0.40              |
| 51:1:2393:U:C2'    | 51:1:2394:C:H5'    | 2.51                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1:2888:C:H2'    | 51:1:2889:C:C6     | 2.56                     | 0.40              |
| 57:A1:224:LEU:HD23 | 57:A2:228:LEU:HD21 | 2.03                     | 0.40              |
| 57:A2:57:THR:HG22  | 57:A2:58:GLU:HG3   | 2.04                     | 0.40              |
| 65:0:574:MET:HE1   | 65:0:601:PHE:CZ    | 2.57                     | 0.40              |
| 65:0:635:LEU:HD23  | 65:0:635:LEU:HA    | 1.98                     | 0.40              |
| 9:I:123:MET:HB2    | 9:I:143:SER:HB3    | 2.04                     | 0.40              |
| 19:S:15:LEU:HB3    | 19:S:54:SER:HB3    | 2.02                     | 0.40              |
| 22:V:11:VAL:HG23   | 22:V:55:GLY:H      | 1.85                     | 0.40              |
| 23:W:25:ILE:HA     | 23:W:28:LEU:HB2    | 2.02                     | 0.40              |
| 26:Z:9:GLU:HB3     | 26:Z:10:PRO:HD3    | 2.03                     | 0.40              |
| 27:b:209:ALA:HA    | 27:b:212:TRP:CE2   | 2.55                     | 0.40              |
| 28:c:56:LYS:HG3    | 28:c:59:ARG:HB3    | 2.04                     | 0.40              |
| 28:c:174:SER:O     | 28:c:174:SER:OG    | 2.37                     | 0.40              |
| 30:e:36:ASN:HB3    | 30:e:152:ASP:HB3   | 2.03                     | 0.40              |
| 32:g:1:MET:HE3     | 32:g:1:MET:HB3     | 1.77                     | 0.40              |
| 35:k:53:LYS:HA     | 35:k:53:LYS:HD3    | 1.96                     | 0.40              |
| 39:o:76:LYS:HE2    | 39:o:76:LYS:HB3    | 1.93                     | 0.40              |
| 51:1:120:U:C2      | 51:1:149:A:C6      | 3.10                     | 0.40              |
| 51:1:164:C:H2'     | 51:1:165:A:O4'     | 2.21                     | 0.40              |
| 51:1:194:G:O6      | 51:1:195:A:C6      | 2.75                     | 0.40              |
| 51:1:221:A:C4      | 51:1:266:G:N7      | 2.90                     | 0.40              |
| 51:1:359:G:H2'     | 51:1:360:U:C5'     | 2.51                     | 0.40              |
| 51:1:706:A:H2'     | 51:1:707:G:C5'     | 2.51                     | 0.40              |
| 51:1:724:U:H2'     | 51:1:725:G:C8      | 2.56                     | 0.40              |
| 51:1:935:C:H2'     | 51:1:936:A:C8      | 2.56                     | 0.40              |
| 51:1:1160:G:C6     | 51:1:1161:C:C4     | 3.09                     | 0.40              |
| 51:1:1279:G:H2'    | 51:1:1280:G:C8     | 2.56                     | 0.40              |
| 51:1:1430:G:H2'    | 51:1:1431:A:O4'    | 2.21                     | 0.40              |
| 51:1:1494:A:C6     | 51:1:1495:A:C6     | 3.09                     | 0.40              |
| 51:1:1749:A:H2'    | 51:1:1750:G:C8     | 2.57                     | 0.40              |
| 51:1:1783:A:N1     | 51:1:2587:A:H2'    | 2.37                     | 0.40              |
| 51:1:1944:U:H3'    | 51:1:1945:G:H5'    | 2.03                     | 0.40              |
| 51:1:2092:U:H5     | 51:1:2199:A:C2     | 2.30                     | 0.40              |
| 51:1:2788:C:H2'    | 51:1:2789:C:C6     | 2.56                     | 0.40              |
| 53:3:195:A:H2'     | 53:3:196:A:C8      | 2.57                     | 0.40              |
| 53:3:1124:G:H1     | 53:3:1149:C:H42    | 1.68                     | 0.40              |
| 56:9:33:DA:H5''    | 58:B1:121:PRO:HG3  | 2.04                     | 0.40              |
| 58:B1:182:ALA:HB1  | 58:B1:238:ILE:CG2  | 2.52                     | 0.40              |
| 58:B1:351:GLY:O    | 58:B1:467:ALA:HA   | 2.21                     | 0.40              |
| 58:B1:1361:THR:N   | 59:B2:1282:GLY:O   | 2.53                     | 0.40              |
| 64:6:69:C:H2'      | 64:6:70:G:C8       | 2.57                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 65:0:418:ILE:HA   | 65:0:486:PRO:HD3   | 2.04                     | 0.40              |
| 65:0:438:LEU:HD21 | 65:0:472:ARG:HD2   | 2.02                     | 0.40              |
| 7:G:161:PHE:HA    | 7:G:183:PHE:HB2    | 2.02                     | 0.40              |
| 15:O:9:ARG:NH2    | 53:3:1279:G:OP1    | 2.53                     | 0.40              |
| 24:X:32:THR:OG1   | 24:X:49:ALA:O      | 2.31                     | 0.40              |
| 29:d:138:LEU:HG   | 29:d:143:LEU:HD12  | 2.03                     | 0.40              |
| 30:e:49:LEU:HD22  | 30:e:83:PRO:HB2    | 2.04                     | 0.40              |
| 31:f:157:LYS:HD3  | 51:1:2658:C:H5''   | 2.02                     | 0.40              |
| 34:j:13:ARG:NH1   | 34:j:49:ASP:O      | 2.41                     | 0.40              |
| 41:q:57:ARG:NH1   | 51:1:1154:G:OP2    | 2.52                     | 0.40              |
| 51:1:55:G:N2      | 51:1:116:C:C2      | 2.90                     | 0.40              |
| 51:1:279:A:N6     | 51:1:361:G:HO2'    | 2.20                     | 0.40              |
| 51:1:367:G:H2'    | 51:1:368:A:C8      | 2.57                     | 0.40              |
| 51:1:510:C:H2'    | 51:1:511:U:H6      | 1.85                     | 0.40              |
| 51:1:914:G:H5'    | 51:1:915:C:OP2     | 2.21                     | 0.40              |
| 51:1:1334:G:C6    | 51:1:1335:C:C4     | 3.09                     | 0.40              |
| 51:1:1695:G:H2'   | 51:1:1696:G:O5'    | 2.22                     | 0.40              |
| 51:1:2093:G:N7    | 51:1:2225:A:H2'    | 2.37                     | 0.40              |
| 51:1:2278:A:C2'   | 51:1:2279:G:H5''   | 2.51                     | 0.40              |
| 51:1:2757:A:H2'   | 51:1:2758:A:H5''   | 2.02                     | 0.40              |
| 53:3:202:G:H2'    | 53:3:203:G:H8      | 1.85                     | 0.40              |
| 53:3:297:G:N2     | 53:3:300:A:OP2     | 2.39                     | 0.40              |
| 53:3:440:C:H2'    | 53:3:441:A:H8      | 1.85                     | 0.40              |
| 53:3:987:G:H2'    | 53:3:988:G:C8      | 2.56                     | 0.40              |
| 54:4:43:G:H5'     | 59:B2:688:GLN:HE22 | 1.85                     | 0.40              |
| 57:A2:104:LYS:HG2 | 57:A2:110:VAL:HG22 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | A     | 64/70 (91%)   | 59 (92%)  | 5 (8%)   | 0        | 100         | 100 |
| 2   | B     | 54/57 (95%)   | 48 (89%)  | 4 (7%)   | 2 (4%)   | 2           | 20  |
| 3   | C     | 48/55 (87%)   | 41 (85%)  | 7 (15%)  | 0        | 100         | 100 |
| 4   | D     | 44/46 (96%)   | 42 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 5   | E     | 62/65 (95%)   | 57 (92%)  | 5 (8%)   | 0        | 100         | 100 |
| 6   | F     | 36/38 (95%)   | 33 (92%)  | 3 (8%)   | 0        | 100         | 100 |
| 7   | G     | 216/241 (90%) | 187 (87%) | 27 (12%) | 2 (1%)   | 14          | 49  |
| 8   | H     | 204/233 (88%) | 194 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 9   | I     | 203/206 (98%) | 172 (85%) | 30 (15%) | 1 (0%)   | 24          | 63  |
| 10  | J     | 155/167 (93%) | 138 (89%) | 17 (11%) | 0        | 100         | 100 |
| 11  | K     | 98/135 (73%)  | 84 (86%)  | 14 (14%) | 0        | 100         | 100 |
| 12  | L     | 149/179 (83%) | 130 (87%) | 19 (13%) | 0        | 100         | 100 |
| 13  | M     | 127/130 (98%) | 118 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 14  | N     | 125/130 (96%) | 104 (83%) | 21 (17%) | 0        | 100         | 100 |
| 15  | O     | 96/103 (93%)  | 87 (91%)  | 8 (8%)   | 1 (1%)   | 12          | 47  |
| 16  | P     | 114/129 (88%) | 100 (88%) | 13 (11%) | 1 (1%)   | 14          | 49  |
| 17  | Q     | 121/124 (98%) | 94 (78%)  | 27 (22%) | 0        | 100         | 100 |
| 18  | R     | 112/118 (95%) | 98 (88%)  | 13 (12%) | 1 (1%)   | 14          | 49  |
| 19  | S     | 98/101 (97%)  | 83 (85%)  | 15 (15%) | 0        | 100         | 100 |
| 20  | T     | 86/89 (97%)   | 75 (87%)  | 11 (13%) | 0        | 100         | 100 |
| 21  | U     | 80/82 (98%)   | 69 (86%)  | 11 (14%) | 0        | 100         | 100 |
| 22  | V     | 78/84 (93%)   | 69 (88%)  | 8 (10%)  | 1 (1%)   | 9           | 41  |
| 23  | W     | 63/75 (84%)   | 56 (89%)  | 5 (8%)   | 2 (3%)   | 3           | 21  |
| 24  | X     | 77/92 (84%)   | 71 (92%)  | 6 (8%)   | 0        | 100         | 100 |
| 25  | Y     | 83/87 (95%)   | 78 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 26  | Z     | 63/71 (89%)   | 44 (70%)  | 18 (29%) | 1 (2%)   | 7           | 37  |
| 27  | b     | 269/273 (98%) | 244 (91%) | 25 (9%)  | 0        | 100         | 100 |
| 28  | c     | 207/209 (99%) | 189 (91%) | 18 (9%)  | 0        | 100         | 100 |
| 29  | d     | 199/201 (99%) | 186 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 30  | e     | 175/179 (98%) | 157 (90%) | 18 (10%) | 0        | 100         | 100 |
| 31  | f     | 174/177 (98%) | 160 (92%) | 14 (8%)  | 0        | 100         | 100 |
| 32  | g     | 50/149 (34%)  | 44 (88%)  | 5 (10%)  | 1 (2%)   | 6           | 31  |

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| Mol | Chain | Analysed          | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|-----------|----------|-------------|-----|
| 33  | i     | 139/142 (98%)     | 110 (79%)  | 26 (19%)  | 3 (2%)   | 5           | 29  |
| 34  | j     | 140/142 (99%)     | 128 (91%)  | 12 (9%)   | 0        | 100         | 100 |
| 35  | k     | 120/123 (98%)     | 106 (88%)  | 14 (12%)  | 0        | 100         | 100 |
| 36  | l     | 141/144 (98%)     | 129 (92%)  | 12 (8%)   | 0        | 100         | 100 |
| 37  | m     | 134/136 (98%)     | 128 (96%)  | 6 (4%)    | 0        | 100         | 100 |
| 38  | n     | 118/127 (93%)     | 103 (87%)  | 15 (13%)  | 0        | 100         | 100 |
| 39  | o     | 114/117 (97%)     | 109 (96%)  | 5 (4%)    | 0        | 100         | 100 |
| 40  | p     | 112/115 (97%)     | 102 (91%)  | 10 (9%)   | 0        | 100         | 100 |
| 41  | q     | 115/118 (98%)     | 110 (96%)  | 3 (3%)    | 2 (2%)   | 7           | 35  |
| 42  | r     | 101/103 (98%)     | 88 (87%)   | 13 (13%)  | 0        | 100         | 100 |
| 43  | s     | 108/110 (98%)     | 101 (94%)  | 7 (6%)    | 0        | 100         | 100 |
| 44  | t     | 91/100 (91%)      | 82 (90%)   | 9 (10%)   | 0        | 100         | 100 |
| 45  | u     | 100/104 (96%)     | 84 (84%)   | 15 (15%)  | 1 (1%)   | 12          | 47  |
| 46  | v     | 92/94 (98%)       | 87 (95%)   | 5 (5%)    | 0        | 100         | 100 |
| 47  | w     | 73/85 (86%)       | 67 (92%)   | 6 (8%)    | 0        | 100         | 100 |
| 48  | x     | 75/78 (96%)       | 72 (96%)   | 2 (3%)    | 1 (1%)   | 9           | 41  |
| 49  | y     | 61/63 (97%)       | 55 (90%)   | 6 (10%)   | 0        | 100         | 100 |
| 50  | z     | 56/59 (95%)       | 52 (93%)   | 4 (7%)    | 0        | 100         | 100 |
| 57  | A1    | 295/329 (90%)     | 273 (92%)  | 21 (7%)   | 1 (0%)   | 36          | 71  |
| 57  | A2    | 282/329 (86%)     | 272 (96%)  | 10 (4%)   | 0        | 100         | 100 |
| 58  | B1    | 1329/1407 (94%)   | 1202 (90%) | 123 (9%)  | 4 (0%)   | 36          | 71  |
| 59  | B2    | 1338/1342 (100%)  | 1203 (90%) | 130 (10%) | 5 (0%)   | 30          | 67  |
| 60  | W0    | 80/91 (88%)       | 77 (96%)   | 3 (4%)    | 0        | 100         | 100 |
| 61  | NA    | 490/495 (99%)     | 474 (97%)  | 14 (3%)   | 2 (0%)   | 30          | 67  |
| 62  | NG    | 150/181 (83%)     | 133 (89%)  | 10 (7%)   | 7 (5%)   | 2           | 17  |
| 65  | 0     | 669/716 (93%)     | 625 (93%)  | 43 (6%)   | 1 (0%)   | 48          | 83  |
| All | All   | 10253/10945 (94%) | 9283 (90%) | 930 (9%)  | 40 (0%)  | 31          | 67  |

All (40) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | x     | 25  | LYS  |
| 58  | B1    | 121 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 61  | NA    | 187  | ARG  |
| 61  | NA    | 188  | PRO  |
| 62  | NG    | 102  | PRO  |
| 62  | NG    | 122  | PRO  |
| 59  | B2    | 43   | PRO  |
| 59  | B2    | 918  | LEU  |
| 62  | NG    | 121  | LYS  |
| 62  | NG    | 163  | SER  |
| 57  | A1    | 250  | ASP  |
| 59  | B2    | 888  | THR  |
| 2   | B     | 23   | ALA  |
| 7   | G     | 19   | THR  |
| 18  | R     | 5    | GLY  |
| 32  | g     | 12   | LEU  |
| 33  | i     | 22   | PRO  |
| 41  | q     | 23   | TYR  |
| 58  | B1    | 43   | THR  |
| 58  | B1    | 193  | ASP  |
| 59  | B2    | 909  | LYS  |
| 7   | G     | 17   | HIS  |
| 15  | O     | 58   | ASN  |
| 22  | V     | 50   | ASN  |
| 23  | W     | 13   | THR  |
| 45  | u     | 97   | SER  |
| 58  | B1    | 1325 | PHE  |
| 9   | I     | 45   | PRO  |
| 23  | W     | 17   | VAL  |
| 33  | i     | 20   | SER  |
| 62  | NG    | 123  | ARG  |
| 62  | NG    | 169  | THR  |
| 62  | NG    | 170  | PRO  |
| 26  | Z     | 10   | PRO  |
| 33  | i     | 23   | VAL  |
| 41  | q     | 6    | GLY  |
| 65  | 0     | 651  | GLY  |
| 59  | B2    | 1317 | PRO  |
| 2   | B     | 24   | VAL  |
| 16  | P     | 88   | 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 |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A     | 58/62 (94%)   | 57 (98%)   | 1 (2%)   | 53          | 67  |
| 2   | B     | 47/48 (98%)   | 47 (100%)  | 0        | 100         | 100 |
| 3   | C     | 45/49 (92%)   | 44 (98%)   | 1 (2%)   | 45          | 64  |
| 4   | D     | 38/38 (100%)  | 37 (97%)   | 1 (3%)   | 40          | 60  |
| 5   | E     | 51/52 (98%)   | 49 (96%)   | 2 (4%)   | 28          | 50  |
| 6   | F     | 34/34 (100%)  | 30 (88%)   | 4 (12%)  | 5           | 19  |
| 7   | G     | 180/199 (90%) | 174 (97%)  | 6 (3%)   | 33          | 55  |
| 8   | H     | 170/190 (90%) | 167 (98%)  | 3 (2%)   | 51          | 67  |
| 9   | I     | 172/173 (99%) | 168 (98%)  | 4 (2%)   | 44          | 63  |
| 10  | J     | 119/126 (94%) | 117 (98%)  | 2 (2%)   | 53          | 67  |
| 11  | K     | 87/116 (75%)  | 82 (94%)   | 5 (6%)   | 18          | 41  |
| 12  | L     | 124/147 (84%) | 124 (100%) | 0        | 100         | 100 |
| 13  | M     | 104/105 (99%) | 103 (99%)  | 1 (1%)   | 68          | 76  |
| 14  | N     | 105/107 (98%) | 95 (90%)   | 10 (10%) | 8           | 26  |
| 15  | O     | 86/90 (96%)   | 78 (91%)   | 8 (9%)   | 8           | 27  |
| 16  | P     | 89/99 (90%)   | 86 (97%)   | 3 (3%)   | 32          | 54  |
| 17  | Q     | 103/104 (99%) | 98 (95%)   | 5 (5%)   | 22          | 44  |
| 18  | R     | 92/96 (96%)   | 91 (99%)   | 1 (1%)   | 65          | 74  |
| 19  | S     | 83/84 (99%)   | 83 (100%)  | 0        | 100         | 100 |
| 20  | T     | 76/77 (99%)   | 73 (96%)   | 3 (4%)   | 28          | 50  |
| 21  | U     | 65/65 (100%)  | 64 (98%)   | 1 (2%)   | 57          | 70  |
| 22  | V     | 74/78 (95%)   | 72 (97%)   | 2 (3%)   | 39          | 59  |
| 23  | W     | 56/65 (86%)   | 52 (93%)   | 4 (7%)   | 13          | 35  |
| 24  | X     | 70/79 (89%)   | 70 (100%)  | 0        | 100         | 100 |
| 25  | Y     | 65/66 (98%)   | 64 (98%)   | 1 (2%)   | 57          | 70  |
| 26  | Z     | 55/61 (90%)   | 47 (86%)   | 8 (14%)  | 3           | 14  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 27  | b     | 216/218 (99%)   | 212 (98%)  | 4 (2%)   | 50          | 66  |
| 28  | c     | 164/164 (100%)  | 164 (100%) | 0        | 100         | 100 |
| 29  | d     | 165/165 (100%)  | 162 (98%)  | 3 (2%)   | 51          | 67  |
| 30  | e     | 148/150 (99%)   | 142 (96%)  | 6 (4%)   | 27          | 49  |
| 31  | f     | 137/138 (99%)   | 132 (96%)  | 5 (4%)   | 31          | 52  |
| 32  | g     | 41/114 (36%)    | 38 (93%)   | 3 (7%)   | 13          | 34  |
| 33  | i     | 109/110 (99%)   | 100 (92%)  | 9 (8%)   | 10          | 31  |
| 34  | j     | 116/116 (100%)  | 116 (100%) | 0        | 100         | 100 |
| 35  | k     | 103/104 (99%)   | 103 (100%) | 0        | 100         | 100 |
| 36  | l     | 102/103 (99%)   | 101 (99%)  | 1 (1%)   | 68          | 76  |
| 37  | m     | 109/109 (100%)  | 103 (94%)  | 6 (6%)   | 19          | 42  |
| 38  | n     | 100/103 (97%)   | 99 (99%)   | 1 (1%)   | 68          | 76  |
| 39  | o     | 86/87 (99%)     | 86 (100%)  | 0        | 100         | 100 |
| 40  | p     | 99/100 (99%)    | 98 (99%)   | 1 (1%)   | 68          | 76  |
| 41  | q     | 89/90 (99%)     | 86 (97%)   | 3 (3%)   | 32          | 54  |
| 42  | r     | 84/84 (100%)    | 82 (98%)   | 2 (2%)   | 43          | 63  |
| 43  | s     | 93/93 (100%)    | 92 (99%)   | 1 (1%)   | 65          | 74  |
| 44  | t     | 80/84 (95%)     | 80 (100%)  | 0        | 100         | 100 |
| 45  | u     | 83/85 (98%)     | 79 (95%)   | 4 (5%)   | 23          | 45  |
| 46  | v     | 78/78 (100%)    | 77 (99%)   | 1 (1%)   | 61          | 72  |
| 47  | w     | 57/63 (90%)     | 57 (100%)  | 0        | 100         | 100 |
| 48  | x     | 67/68 (98%)     | 67 (100%)  | 0        | 100         | 100 |
| 49  | y     | 55/55 (100%)    | 55 (100%)  | 0        | 100         | 100 |
| 50  | z     | 48/49 (98%)     | 46 (96%)   | 2 (4%)   | 26          | 48  |
| 57  | A1    | 185/286 (65%)   | 174 (94%)  | 11 (6%)  | 18          | 40  |
| 57  | A2    | 186/286 (65%)   | 184 (99%)  | 2 (1%)   | 65          | 74  |
| 58  | B1    | 1110/1168 (95%) | 1017 (92%) | 93 (8%)  | 10          | 30  |
| 59  | B2    | 1150/1157 (99%) | 1118 (97%) | 32 (3%)  | 38          | 59  |
| 60  | W0    | 70/75 (93%)     | 69 (99%)   | 1 (1%)   | 59          | 71  |
| 65  | 0     | 553/588 (94%)   | 482 (87%)  | 71 (13%) | 4           | 17  |
| All | All   | 7931/8500 (93%) | 7593 (96%) | 338 (4%) | 27          | 48  |

All (338) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 21  | VAL  |
| 3   | C     | 22  | THR  |
| 4   | D     | 44  | VAL  |
| 5   | E     | 28  | LEU  |
| 5   | E     | 31  | ILE  |
| 6   | F     | 34  | LYS  |
| 6   | F     | 35  | GLN  |
| 6   | F     | 36  | ARG  |
| 6   | F     | 37  | GLN  |
| 7   | G     | 8   | MET  |
| 7   | G     | 10  | LYS  |
| 7   | G     | 13  | VAL  |
| 7   | G     | 14  | HIS  |
| 7   | G     | 17  | HIS  |
| 7   | G     | 29  | PHE  |
| 8   | H     | 74  | ILE  |
| 8   | H     | 156 | LEU  |
| 8   | H     | 164 | THR  |
| 9   | I     | 44  | LYS  |
| 9   | I     | 46  | ARG  |
| 9   | I     | 96  | ARG  |
| 9   | I     | 97  | LEU  |
| 10  | J     | 55  | VAL  |
| 10  | J     | 130 | THR  |
| 11  | K     | 89  | VAL  |
| 11  | K     | 90  | MET  |
| 11  | K     | 91  | ARG  |
| 11  | K     | 92  | THR  |
| 11  | K     | 94  | HIS  |
| 13  | M     | 102 | VAL  |
| 14  | N     | 40  | ARG  |
| 14  | N     | 44  | ARG  |
| 14  | N     | 45  | MET  |
| 14  | N     | 52  | GLU  |
| 14  | N     | 53  | LEU  |
| 14  | N     | 54  | VAL  |
| 14  | N     | 57  | VAL  |
| 14  | N     | 59  | LYS  |
| 14  | N     | 60  | LEU  |
| 14  | N     | 65  | THR  |
| 15  | O     | 16  | ARG  |
| 15  | O     | 82  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | O     | 83  | THR  |
| 15  | O     | 87  | LEU  |
| 15  | O     | 88  | MET  |
| 15  | O     | 89  | ARG  |
| 15  | O     | 91  | ASP  |
| 15  | O     | 92  | LEU  |
| 16  | P     | 120 | CYS  |
| 16  | P     | 121 | ARG  |
| 16  | P     | 124 | LYS  |
| 17  | Q     | 15  | VAL  |
| 17  | Q     | 17  | LYS  |
| 17  | Q     | 20  | VAL  |
| 17  | Q     | 29  | LYS  |
| 17  | Q     | 34  | THR  |
| 18  | R     | 64  | VAL  |
| 20  | T     | 82  | GLU  |
| 20  | T     | 86  | LEU  |
| 20  | T     | 88  | ARG  |
| 21  | U     | 36  | VAL  |
| 22  | V     | 47  | ASP  |
| 22  | V     | 52  | CYS  |
| 23  | W     | 15  | GLU  |
| 23  | W     | 17  | VAL  |
| 23  | W     | 18  | GLN  |
| 23  | W     | 70  | THR  |
| 25  | Y     | 85  | LEU  |
| 26  | Z     | 3   | ILE  |
| 26  | Z     | 4   | LYS  |
| 26  | Z     | 5   | VAL  |
| 26  | Z     | 12  | ASP  |
| 26  | Z     | 15  | LEU  |
| 26  | Z     | 19  | LYS  |
| 26  | Z     | 20  | ARG  |
| 26  | Z     | 27  | VAL  |
| 27  | b     | 129 | LEU  |
| 27  | b     | 131 | MET  |
| 27  | b     | 132 | ARG  |
| 27  | b     | 203 | VAL  |
| 29  | d     | 14  | VAL  |
| 29  | d     | 118 | LEU  |
| 29  | d     | 198 | GLU  |
| 30  | e     | 39  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | e     | 77  | LYS  |
| 30  | e     | 78  | ILE  |
| 30  | e     | 79  | ARG  |
| 30  | e     | 174 | PHE  |
| 30  | e     | 177 | ARG  |
| 31  | f     | 9   | VAL  |
| 31  | f     | 131 | VAL  |
| 31  | f     | 172 | GLU  |
| 31  | f     | 174 | LYS  |
| 31  | f     | 176 | LYS  |
| 32  | g     | 4   | ILE  |
| 32  | g     | 5   | LEU  |
| 32  | g     | 9   | VAL  |
| 33  | i     | 18  | ASN  |
| 33  | i     | 20  | SER  |
| 33  | i     | 22  | PRO  |
| 33  | i     | 23  | VAL  |
| 33  | i     | 27  | LEU  |
| 33  | i     | 29  | GLN  |
| 33  | i     | 34  | ILE  |
| 33  | i     | 35  | MET  |
| 33  | i     | 36  | GLU  |
| 36  | l     | 85  | VAL  |
| 37  | m     | 44  | ARG  |
| 37  | m     | 47  | GLU  |
| 37  | m     | 50  | ARG  |
| 37  | m     | 55  | ARG  |
| 37  | m     | 58  | LYS  |
| 37  | m     | 59  | ARG  |
| 38  | n     | 13  | ASN  |
| 40  | p     | 52  | ARG  |
| 41  | q     | 4   | LYS  |
| 41  | q     | 5   | ARG  |
| 41  | q     | 28  | SER  |
| 42  | r     | 53  | PHE  |
| 42  | r     | 54  | VAL  |
| 43  | s     | 3   | THR  |
| 45  | u     | 35  | VAL  |
| 45  | u     | 93  | ARG  |
| 45  | u     | 100 | GLU  |
| 45  | u     | 101 | THR  |
| 46  | v     | 72  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | z     | 16  | LEU  |
| 50  | z     | 40  | THR  |
| 57  | A1    | 9   | LEU  |
| 57  | A1    | 12  | ARG  |
| 57  | A1    | 13  | LEU  |
| 57  | A1    | 18  | GLN  |
| 57  | A1    | 19  | VAL  |
| 57  | A1    | 22  | THR  |
| 57  | A1    | 27  | THR  |
| 57  | A1    | 28  | LEU  |
| 57  | A1    | 33  | ARG  |
| 57  | A1    | 46  | ILE  |
| 57  | A1    | 48  | LEU  |
| 57  | A2    | 29  | GLU  |
| 57  | A2    | 74  | VAL  |
| 58  | B1    | 24  | LEU  |
| 58  | B1    | 40  | LYS  |
| 58  | B1    | 42  | GLU  |
| 58  | B1    | 44  | ILE  |
| 58  | B1    | 47  | ARG  |
| 58  | B1    | 49  | PHE  |
| 58  | B1    | 50  | LYS  |
| 58  | B1    | 60  | ARG  |
| 58  | B1    | 66  | LYS  |
| 58  | B1    | 69  | GLU  |
| 58  | B1    | 71  | LEU  |
| 58  | B1    | 74  | LYS  |
| 58  | B1    | 76  | LYS  |
| 58  | B1    | 78  | LEU  |
| 58  | B1    | 80  | HIS  |
| 58  | B1    | 81  | ARG  |
| 58  | B1    | 87  | LYS  |
| 58  | B1    | 91  | GLU  |
| 58  | B1    | 93  | THR  |
| 58  | B1    | 94  | GLN  |
| 58  | B1    | 95  | THR  |
| 58  | B1    | 96  | LYS  |
| 58  | B1    | 99  | ARG  |
| 58  | B1    | 100 | GLU  |
| 58  | B1    | 114 | ILE  |
| 58  | B1    | 117 | LEU  |
| 58  | B1    | 120 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58  | B1    | 126 | LEU  |
| 58  | B1    | 132 | LEU  |
| 58  | B1    | 135 | ILE  |
| 58  | B1    | 142 | GLU  |
| 58  | B1    | 144 | TYR  |
| 58  | B1    | 145 | VAL  |
| 58  | B1    | 146 | VAL  |
| 58  | B1    | 147 | ILE  |
| 58  | B1    | 152 | THR  |
| 58  | B1    | 154 | LEU  |
| 58  | B1    | 157 | GLN  |
| 58  | B1    | 159 | ILE  |
| 58  | B1    | 172 | PHE  |
| 58  | B1    | 174 | ASP  |
| 58  | B1    | 175 | GLU  |
| 58  | B1    | 180 | MET  |
| 58  | B1    | 190 | LYS  |
| 58  | B1    | 193 | ASP  |
| 58  | B1    | 196 | GLN  |
| 58  | B1    | 210 | SER  |
| 58  | B1    | 212 | THR  |
| 58  | B1    | 216 | LYS  |
| 58  | B1    | 222 | LYS  |
| 58  | B1    | 223 | LEU  |
| 58  | B1    | 227 | PHE  |
| 58  | B1    | 233 | LYS  |
| 58  | B1    | 237 | MET  |
| 58  | B1    | 238 | ILE  |
| 58  | B1    | 239 | LEU  |
| 58  | B1    | 240 | THR  |
| 58  | B1    | 244 | VAL  |
| 58  | B1    | 255 | LEU  |
| 58  | B1    | 256 | ASP  |
| 58  | B1    | 259 | ARG  |
| 58  | B1    | 281 | ARG  |
| 58  | B1    | 282 | LEU  |
| 58  | B1    | 285 | LEU  |
| 58  | B1    | 290 | ILE  |
| 58  | B1    | 317 | THR  |
| 58  | B1    | 322 | ARG  |
| 58  | B1    | 324 | LEU  |
| 58  | B1    | 363 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 58  | B1    | 385  | LEU  |
| 58  | B1    | 386  | GLU  |
| 58  | B1    | 387  | LEU  |
| 58  | B1    | 390  | LEU  |
| 58  | B1    | 393  | THR  |
| 58  | B1    | 394  | ILE  |
| 58  | B1    | 395  | LYS  |
| 58  | B1    | 416  | ILE  |
| 58  | B1    | 417  | ARG  |
| 58  | B1    | 425  | ARG  |
| 58  | B1    | 506  | VAL  |
| 58  | B1    | 514  | THR  |
| 58  | B1    | 800  | LEU  |
| 58  | B1    | 807  | LEU  |
| 58  | B1    | 839  | VAL  |
| 58  | B1    | 901  | ARG  |
| 58  | B1    | 903  | LEU  |
| 58  | B1    | 1172 | LYS  |
| 58  | B1    | 1181 | ASP  |
| 58  | B1    | 1233 | ILE  |
| 58  | B1    | 1327 | GLU  |
| 58  | B1    | 1328 | THR  |
| 58  | B1    | 1331 | VAL  |
| 58  | B1    | 1332 | LEU  |
| 59  | B2    | 44   | GLU  |
| 59  | B2    | 49   | LEU  |
| 59  | B2    | 56   | VAL  |
| 59  | B2    | 146  | VAL  |
| 59  | B2    | 483  | ASP  |
| 59  | B2    | 487  | LEU  |
| 59  | B2    | 516  | ASP  |
| 59  | B2    | 538  | LEU  |
| 59  | B2    | 540  | ARG  |
| 59  | B2    | 545  | PHE  |
| 59  | B2    | 546  | GLU  |
| 59  | B2    | 615  | VAL  |
| 59  | B2    | 857  | VAL  |
| 59  | B2    | 859  | GLU  |
| 59  | B2    | 887  | VAL  |
| 59  | B2    | 890  | LYS  |
| 59  | B2    | 892  | GLU  |
| 59  | B2    | 894  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 59  | B2    | 900  | LYS  |
| 59  | B2    | 901  | LEU  |
| 59  | B2    | 902  | LEU  |
| 59  | B2    | 903  | ARG  |
| 59  | B2    | 905  | ILE  |
| 59  | B2    | 906  | PHE  |
| 59  | B2    | 909  | LYS  |
| 59  | B2    | 913  | VAL  |
| 59  | B2    | 915  | ASP  |
| 59  | B2    | 918  | LEU  |
| 59  | B2    | 920  | VAL  |
| 59  | B2    | 922  | ASN  |
| 59  | B2    | 1076 | ILE  |
| 59  | B2    | 1151 | LEU  |
| 60  | W0    | 63   | ILE  |
| 65  | 0     | 3    | ARG  |
| 65  | 0     | 19   | ILE  |
| 65  | 0     | 23   | LYS  |
| 65  | 0     | 24   | THR  |
| 65  | 0     | 28   | GLU  |
| 65  | 0     | 93   | VAL  |
| 65  | 0     | 96   | THR  |
| 65  | 0     | 98   | GLU  |
| 65  | 0     | 104  | ARG  |
| 65  | 0     | 105  | VAL  |
| 65  | 0     | 143  | LYS  |
| 65  | 0     | 144  | MET  |
| 65  | 0     | 147  | MET  |
| 65  | 0     | 254  | GLN  |
| 65  | 0     | 273  | LYS  |
| 65  | 0     | 343  | VAL  |
| 65  | 0     | 358  | GLU  |
| 65  | 0     | 365  | GLN  |
| 65  | 0     | 366  | MET  |
| 65  | 0     | 369  | ASN  |
| 65  | 0     | 370  | LYS  |
| 65  | 0     | 371  | ARG  |
| 65  | 0     | 372  | GLU  |
| 65  | 0     | 377  | VAL  |
| 65  | 0     | 378  | ARG  |
| 65  | 0     | 425  | LYS  |
| 65  | 0     | 429  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65  | 0     | 430 | LYS  |
| 65  | 0     | 431 | MET  |
| 65  | 0     | 433 | LEU  |
| 65  | 0     | 437 | ARG  |
| 65  | 0     | 461 | MET  |
| 65  | 0     | 464 | LEU  |
| 65  | 0     | 471 | ASP  |
| 65  | 0     | 472 | ARG  |
| 65  | 0     | 473 | MET  |
| 65  | 0     | 476 | GLU  |
| 65  | 0     | 478 | ASN  |
| 65  | 0     | 485 | LYS  |
| 65  | 0     | 487 | GLN  |
| 65  | 0     | 488 | VAL  |
| 65  | 0     | 495 | ARG  |
| 65  | 0     | 504 | LYS  |
| 65  | 0     | 512 | ARG  |
| 65  | 0     | 514 | GLN  |
| 65  | 0     | 539 | ASP  |
| 65  | 0     | 580 | PHE  |
| 65  | 0     | 591 | LEU  |
| 65  | 0     | 594 | LYS  |
| 65  | 0     | 595 | LEU  |
| 65  | 0     | 613 | LEU  |
| 65  | 0     | 626 | GLU  |
| 65  | 0     | 630 | ASP  |
| 65  | 0     | 642 | LEU  |
| 65  | 0     | 643 | LYS  |
| 65  | 0     | 645 | GLN  |
| 65  | 0     | 646 | GLU  |
| 65  | 0     | 648 | GLU  |
| 65  | 0     | 649 | VAL  |
| 65  | 0     | 650 | THR  |
| 65  | 0     | 654 | ILE  |
| 65  | 0     | 668 | THR  |
| 65  | 0     | 671 | ARG  |
| 65  | 0     | 677 | ARG  |
| 65  | 0     | 686 | LYS  |
| 65  | 0     | 687 | TYR  |
| 65  | 0     | 688 | ASP  |
| 65  | 0     | 689 | GLU  |
| 65  | 0     | 693 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65  | 0     | 702 | ARG  |
| 65  | 0     | 704 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | ASN  |
| 1   | A     | 33  | ASN  |
| 1   | A     | 61  | ASN  |
| 2   | B     | 4   | GLN  |
| 3   | C     | 25  | ASN  |
| 3   | C     | 44  | GLN  |
| 4   | D     | 16  | HIS  |
| 6   | F     | 35  | GLN  |
| 6   | F     | 37  | GLN  |
| 7   | G     | 14  | HIS  |
| 7   | G     | 108 | GLN  |
| 7   | G     | 119 | GLN  |
| 7   | G     | 121 | GLN  |
| 7   | G     | 167 | HIS  |
| 8   | H     | 7   | ASN  |
| 8   | H     | 68  | HIS  |
| 8   | H     | 99  | GLN  |
| 8   | H     | 122 | GLN  |
| 8   | H     | 138 | GLN  |
| 8   | H     | 139 | ASN  |
| 9   | I     | 197 | HIS  |
| 10  | J     | 76  | ASN  |
| 10  | J     | 88  | HIS  |
| 10  | J     | 121 | ASN  |
| 12  | L     | 85  | GLN  |
| 12  | L     | 121 | ASN  |
| 12  | L     | 147 | ASN  |
| 13  | M     | 3   | GLN  |
| 13  | M     | 37  | ASN  |
| 13  | M     | 66  | GLN  |
| 14  | N     | 4   | GLN  |
| 14  | N     | 30  | ASN  |
| 15  | O     | 20  | GLN  |
| 15  | O     | 58  | ASN  |
| 16  | P     | 80  | ASN  |
| 17  | Q     | 4   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | Q     | 71  | HIS  |
| 18  | R     | 7   | ASN  |
| 18  | R     | 99  | GLN  |
| 19  | S     | 59  | GLN  |
| 20  | T     | 19  | ASN  |
| 20  | T     | 39  | GLN  |
| 22  | V     | 30  | HIS  |
| 24  | X     | 68  | HIS  |
| 25  | Y     | 2   | ASN  |
| 25  | Y     | 77  | ASN  |
| 26  | Z     | 8   | ASN  |
| 27  | b     | 24  | HIS  |
| 27  | b     | 69  | ASN  |
| 27  | b     | 89  | ASN  |
| 27  | b     | 142 | ASN  |
| 27  | b     | 259 | ASN  |
| 28  | c     | 49  | GLN  |
| 28  | c     | 134 | HIS  |
| 28  | c     | 150 | GLN  |
| 28  | c     | 164 | GLN  |
| 29  | d     | 41  | GLN  |
| 29  | d     | 62  | GLN  |
| 29  | d     | 90  | GLN  |
| 29  | d     | 94  | GLN  |
| 29  | d     | 165 | HIS  |
| 30  | e     | 4   | HIS  |
| 31  | f     | 47  | ASN  |
| 31  | f     | 87  | GLN  |
| 32  | g     | 2   | GLN  |
| 33  | i     | 30  | GLN  |
| 34  | j     | 58  | ASN  |
| 34  | j     | 135 | GLN  |
| 35  | k     | 3   | GLN  |
| 35  | k     | 5   | GLN  |
| 36  | l     | 4   | ASN  |
| 36  | l     | 104 | GLN  |
| 37  | m     | 13  | HIS  |
| 38  | n     | 13  | ASN  |
| 40  | p     | 2   | ASN  |
| 40  | p     | 114 | ASN  |
| 41  | q     | 55  | GLN  |
| 41  | q     | 58  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | r     | 18   | GLN  |
| 42  | r     | 82   | HIS  |
| 43  | s     | 7    | HIS  |
| 44  | t     | 28   | ASN  |
| 44  | t     | 59   | ASN  |
| 44  | t     | 92   | ASN  |
| 45  | u     | 52   | ASN  |
| 46  | v     | 75   | GLN  |
| 46  | v     | 87   | GLN  |
| 47  | w     | 53   | HIS  |
| 48  | x     | 16   | ASN  |
| 48  | x     | 33   | HIS  |
| 49  | y     | 31   | GLN  |
| 49  | y     | 38   | GLN  |
| 49  | y     | 41   | HIS  |
| 49  | y     | 45   | GLN  |
| 50  | z     | 8    | GLN  |
| 57  | A1    | 37   | HIS  |
| 57  | A1    | 66   | HIS  |
| 57  | A1    | 84   | ASN  |
| 57  | A1    | 117  | HIS  |
| 57  | A1    | 227  | GLN  |
| 57  | A2    | 23   | HIS  |
| 57  | A2    | 227  | GLN  |
| 58  | B1    | 45   | ASN  |
| 58  | B1    | 196  | GLN  |
| 58  | B1    | 364  | HIS  |
| 58  | B1    | 424  | ASN  |
| 58  | B1    | 469  | HIS  |
| 58  | B1    | 805  | GLN  |
| 58  | B1    | 865  | HIS  |
| 58  | B1    | 1195 | GLN  |
| 58  | B1    | 1238 | GLN  |
| 58  | B1    | 1259 | GLN  |
| 59  | B2    | 69   | GLN  |
| 59  | B2    | 314  | ASN  |
| 59  | B2    | 330  | HIS  |
| 59  | B2    | 343  | HIS  |
| 59  | B2    | 518  | ASN  |
| 59  | B2    | 554  | HIS  |
| 59  | B2    | 688  | GLN  |
| 59  | B2    | 808  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 59  | B2    | 965  | GLN  |
| 59  | B2    | 1008 | GLN  |
| 59  | B2    | 1080 | ASN  |
| 59  | B2    | 1237 | HIS  |
| 59  | B2    | 1268 | GLN  |
| 59  | B2    | 1313 | HIS  |
| 60  | W0    | 7    | GLN  |
| 60  | W0    | 31   | GLN  |
| 60  | W0    | 62   | GLN  |
| 65  | 0     | 344  | ASN  |
| 65  | 0     | 367  | HIS  |
| 65  | 0     | 465  | HIS  |
| 65  | 0     | 496  | GLN  |
| 65  | 0     | 514  | GLN  |
| 65  | 0     | 579  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 51  | 1     | 2902/2904 (99%) | 398 (13%)         | 16 (0%)         |
| 52  | 2     | 119/120 (99%)   | 17 (14%)          | 1 (0%)          |
| 53  | 3     | 1538/1542 (99%) | 253 (16%)         | 4 (0%)          |
| 54  | 4     | 37/44 (84%)     | 21 (56%)          | 2 (5%)          |
| 63  | 5     | 75/76 (98%)     | 39 (52%)          | 6 (8%)          |
| 64  | 6     | 76/77 (98%)     | 27 (35%)          | 2 (2%)          |
| All | All   | 4747/4763 (99%) | 755 (15%)         | 31 (0%)         |

All (755) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 1     | 10  | A    |
| 51  | 1     | 12  | U    |
| 51  | 1     | 34  | U    |
| 51  | 1     | 35  | G    |
| 51  | 1     | 46  | G    |
| 51  | 1     | 51  | G    |
| 51  | 1     | 55  | G    |
| 51  | 1     | 63  | A    |
| 51  | 1     | 71  | A    |
| 51  | 1     | 74  | A    |
| 51  | 1     | 75  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 1     | 102 | U    |
| 51  | 1     | 103 | A    |
| 51  | 1     | 119 | A    |
| 51  | 1     | 120 | U    |
| 51  | 1     | 139 | U    |
| 51  | 1     | 140 | C    |
| 51  | 1     | 141 | G    |
| 51  | 1     | 149 | A    |
| 51  | 1     | 162 | U    |
| 51  | 1     | 163 | C    |
| 51  | 1     | 178 | G    |
| 51  | 1     | 196 | A    |
| 51  | 1     | 199 | A    |
| 51  | 1     | 216 | A    |
| 51  | 1     | 221 | A    |
| 51  | 1     | 222 | A    |
| 51  | 1     | 229 | C    |
| 51  | 1     | 248 | G    |
| 51  | 1     | 255 | A    |
| 51  | 1     | 265 | A    |
| 51  | 1     | 266 | G    |
| 51  | 1     | 276 | U    |
| 51  | 1     | 281 | C    |
| 51  | 1     | 285 | G    |
| 51  | 1     | 294 | A    |
| 51  | 1     | 323 | C    |
| 51  | 1     | 329 | G    |
| 51  | 1     | 330 | A    |
| 51  | 1     | 353 | C    |
| 51  | 1     | 361 | G    |
| 51  | 1     | 362 | A    |
| 51  | 1     | 371 | A    |
| 51  | 1     | 372 | G    |
| 51  | 1     | 386 | G    |
| 51  | 1     | 387 | U    |
| 51  | 1     | 396 | G    |
| 51  | 1     | 404 | A    |
| 51  | 1     | 406 | G    |
| 51  | 1     | 411 | G    |
| 51  | 1     | 424 | G    |
| 51  | 1     | 451 | U    |
| 51  | 1     | 457 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 1     | 481 | G    |
| 51  | 1     | 482 | A    |
| 51  | 1     | 491 | G    |
| 51  | 1     | 504 | A    |
| 51  | 1     | 505 | A    |
| 51  | 1     | 526 | A    |
| 51  | 1     | 529 | A    |
| 51  | 1     | 531 | C    |
| 51  | 1     | 532 | A    |
| 51  | 1     | 533 | G    |
| 51  | 1     | 544 | C    |
| 51  | 1     | 545 | U    |
| 51  | 1     | 546 | U    |
| 51  | 1     | 547 | A    |
| 51  | 1     | 562 | U    |
| 51  | 1     | 563 | A    |
| 51  | 1     | 573 | U    |
| 51  | 1     | 574 | A    |
| 51  | 1     | 575 | A    |
| 51  | 1     | 603 | A    |
| 51  | 1     | 614 | A    |
| 51  | 1     | 616 | A    |
| 51  | 1     | 627 | A    |
| 51  | 1     | 637 | A    |
| 51  | 1     | 646 | U    |
| 51  | 1     | 647 | G    |
| 51  | 1     | 654 | A    |
| 51  | 1     | 669 | G    |
| 51  | 1     | 671 | C    |
| 51  | 1     | 677 | A    |
| 51  | 1     | 686 | U    |
| 51  | 1     | 687 | C    |
| 51  | 1     | 695 | G    |
| 51  | 1     | 730 | A    |
| 51  | 1     | 745 | G    |
| 51  | 1     | 747 | C    |
| 51  | 1     | 758 | C    |
| 51  | 1     | 764 | A    |
| 51  | 1     | 765 | C    |
| 51  | 1     | 775 | G    |
| 51  | 1     | 782 | A    |
| 51  | 1     | 784 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 785  | G    |
| 51  | 1     | 789  | A    |
| 51  | 1     | 791  | C    |
| 51  | 1     | 792  | A    |
| 51  | 1     | 801  | G    |
| 51  | 1     | 805  | G    |
| 51  | 1     | 812  | C    |
| 51  | 1     | 819  | A    |
| 51  | 1     | 827  | U    |
| 51  | 1     | 828  | U    |
| 51  | 1     | 829  | A    |
| 51  | 1     | 830  | G    |
| 51  | 1     | 845  | A    |
| 51  | 1     | 846  | U    |
| 51  | 1     | 858  | G    |
| 51  | 1     | 860  | U    |
| 51  | 1     | 878  | A    |
| 51  | 1     | 887  | U    |
| 51  | 1     | 896  | A    |
| 51  | 1     | 910  | A    |
| 51  | 1     | 911  | A    |
| 51  | 1     | 932  | U    |
| 51  | 1     | 941  | A    |
| 51  | 1     | 946  | C    |
| 51  | 1     | 961  | C    |
| 51  | 1     | 968  | C    |
| 51  | 1     | 974  | G    |
| 51  | 1     | 981  | A    |
| 51  | 1     | 983  | A    |
| 51  | 1     | 985  | C    |
| 51  | 1     | 995  | C    |
| 51  | 1     | 996  | A    |
| 51  | 1     | 1005 | C    |
| 51  | 1     | 1012 | U    |
| 51  | 1     | 1013 | C    |
| 51  | 1     | 1021 | A    |
| 51  | 1     | 1022 | G    |
| 51  | 1     | 1031 | G    |
| 51  | 1     | 1033 | U    |
| 51  | 1     | 1045 | C    |
| 51  | 1     | 1046 | A    |
| 51  | 1     | 1047 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 1057 | A    |
| 51  | 1     | 1058 | U    |
| 51  | 1     | 1060 | U    |
| 51  | 1     | 1061 | U    |
| 51  | 1     | 1063 | G    |
| 51  | 1     | 1065 | U    |
| 51  | 1     | 1066 | U    |
| 51  | 1     | 1068 | G    |
| 51  | 1     | 1069 | A    |
| 51  | 1     | 1070 | A    |
| 51  | 1     | 1071 | G    |
| 51  | 1     | 1073 | A    |
| 51  | 1     | 1075 | C    |
| 51  | 1     | 1078 | U    |
| 51  | 1     | 1083 | U    |
| 51  | 1     | 1084 | A    |
| 51  | 1     | 1086 | A    |
| 51  | 1     | 1088 | A    |
| 51  | 1     | 1104 | C    |
| 51  | 1     | 1111 | A    |
| 51  | 1     | 1131 | G    |
| 51  | 1     | 1132 | U    |
| 51  | 1     | 1133 | A    |
| 51  | 1     | 1135 | C    |
| 51  | 1     | 1139 | G    |
| 51  | 1     | 1142 | A    |
| 51  | 1     | 1143 | A    |
| 51  | 1     | 1157 | G    |
| 51  | 1     | 1175 | A    |
| 51  | 1     | 1177 | G    |
| 51  | 1     | 1178 | C    |
| 51  | 1     | 1180 | U    |
| 51  | 1     | 1186 | G    |
| 51  | 1     | 1212 | G    |
| 51  | 1     | 1225 | G    |
| 51  | 1     | 1253 | A    |
| 51  | 1     | 1256 | G    |
| 51  | 1     | 1271 | G    |
| 51  | 1     | 1272 | A    |
| 51  | 1     | 1273 | U    |
| 51  | 1     | 1289 | C    |
| 51  | 1     | 1294 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 1300 | G    |
| 51  | 1     | 1301 | A    |
| 51  | 1     | 1345 | C    |
| 51  | 1     | 1352 | U    |
| 51  | 1     | 1365 | A    |
| 51  | 1     | 1378 | A    |
| 51  | 1     | 1379 | U    |
| 51  | 1     | 1383 | A    |
| 51  | 1     | 1406 | U    |
| 51  | 1     | 1416 | G    |
| 51  | 1     | 1419 | A    |
| 51  | 1     | 1420 | A    |
| 51  | 1     | 1427 | A    |
| 51  | 1     | 1429 | G    |
| 51  | 1     | 1452 | G    |
| 51  | 1     | 1453 | A    |
| 51  | 1     | 1461 | C    |
| 51  | 1     | 1482 | G    |
| 51  | 1     | 1490 | A    |
| 51  | 1     | 1491 | G    |
| 51  | 1     | 1497 | U    |
| 51  | 1     | 1504 | A    |
| 51  | 1     | 1515 | A    |
| 51  | 1     | 1524 | G    |
| 51  | 1     | 1533 | C    |
| 51  | 1     | 1535 | A    |
| 51  | 1     | 1536 | C    |
| 51  | 1     | 1537 | G    |
| 51  | 1     | 1555 | G    |
| 51  | 1     | 1560 | G    |
| 51  | 1     | 1565 | C    |
| 51  | 1     | 1569 | A    |
| 51  | 1     | 1578 | U    |
| 51  | 1     | 1583 | A    |
| 51  | 1     | 1608 | A    |
| 51  | 1     | 1616 | A    |
| 51  | 1     | 1634 | A    |
| 51  | 1     | 1647 | U    |
| 51  | 1     | 1648 | U    |
| 51  | 1     | 1674 | G    |
| 51  | 1     | 1698 | A    |
| 51  | 1     | 1699 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 1703 | G    |
| 51  | 1     | 1715 | G    |
| 51  | 1     | 1716 | U    |
| 51  | 1     | 1729 | U    |
| 51  | 1     | 1730 | C    |
| 51  | 1     | 1732 | C    |
| 51  | 1     | 1738 | G    |
| 51  | 1     | 1758 | U    |
| 51  | 1     | 1764 | C    |
| 51  | 1     | 1773 | A    |
| 51  | 1     | 1783 | A    |
| 51  | 1     | 1784 | A    |
| 51  | 1     | 1786 | A    |
| 51  | 1     | 1800 | C    |
| 51  | 1     | 1801 | A    |
| 51  | 1     | 1802 | A    |
| 51  | 1     | 1808 | A    |
| 51  | 1     | 1809 | A    |
| 51  | 1     | 1816 | C    |
| 51  | 1     | 1829 | A    |
| 51  | 1     | 1833 | C    |
| 51  | 1     | 1834 | U    |
| 51  | 1     | 1870 | C    |
| 51  | 1     | 1871 | A    |
| 51  | 1     | 1901 | A    |
| 51  | 1     | 1906 | G    |
| 51  | 1     | 1913 | A    |
| 51  | 1     | 1914 | C    |
| 51  | 1     | 1929 | G    |
| 51  | 1     | 1931 | U    |
| 51  | 1     | 1936 | A    |
| 51  | 1     | 1937 | A    |
| 51  | 1     | 1938 | A    |
| 51  | 1     | 1939 | U    |
| 51  | 1     | 1943 | U    |
| 51  | 1     | 1955 | U    |
| 51  | 1     | 1967 | C    |
| 51  | 1     | 1970 | A    |
| 51  | 1     | 1971 | U    |
| 51  | 1     | 1972 | G    |
| 51  | 1     | 1990 | C    |
| 51  | 1     | 1993 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 1997 | C    |
| 51  | 1     | 2020 | A    |
| 51  | 1     | 2022 | U    |
| 51  | 1     | 2023 | C    |
| 51  | 1     | 2024 | G    |
| 51  | 1     | 2027 | G    |
| 51  | 1     | 2030 | A    |
| 51  | 1     | 2031 | A    |
| 51  | 1     | 2033 | A    |
| 51  | 1     | 2034 | U    |
| 51  | 1     | 2043 | C    |
| 51  | 1     | 2052 | A    |
| 51  | 1     | 2055 | C    |
| 51  | 1     | 2056 | G    |
| 51  | 1     | 2060 | A    |
| 51  | 1     | 2061 | G    |
| 51  | 1     | 2069 | G    |
| 51  | 1     | 2093 | G    |
| 51  | 1     | 2096 | C    |
| 51  | 1     | 2100 | G    |
| 51  | 1     | 2110 | G    |
| 51  | 1     | 2111 | U    |
| 51  | 1     | 2118 | U    |
| 51  | 1     | 2119 | A    |
| 51  | 1     | 2123 | G    |
| 51  | 1     | 2128 | G    |
| 51  | 1     | 2131 | U    |
| 51  | 1     | 2132 | U    |
| 51  | 1     | 2133 | G    |
| 51  | 1     | 2134 | A    |
| 51  | 1     | 2137 | U    |
| 51  | 1     | 2141 | G    |
| 51  | 1     | 2145 | C    |
| 51  | 1     | 2149 | U    |
| 51  | 1     | 2162 | G    |
| 51  | 1     | 2164 | C    |
| 51  | 1     | 2166 | U    |
| 51  | 1     | 2172 | U    |
| 51  | 1     | 2173 | A    |
| 51  | 1     | 2174 | C    |
| 51  | 1     | 2189 | U    |
| 51  | 1     | 2192 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 2198 | A    |
| 51  | 1     | 2204 | G    |
| 51  | 1     | 2211 | A    |
| 51  | 1     | 2213 | U    |
| 51  | 1     | 2225 | A    |
| 51  | 1     | 2238 | G    |
| 51  | 1     | 2239 | G    |
| 51  | 1     | 2243 | U    |
| 51  | 1     | 2268 | A    |
| 51  | 1     | 2275 | C    |
| 51  | 1     | 2279 | G    |
| 51  | 1     | 2283 | C    |
| 51  | 1     | 2287 | A    |
| 51  | 1     | 2288 | A    |
| 51  | 1     | 2305 | U    |
| 51  | 1     | 2309 | A    |
| 51  | 1     | 2325 | G    |
| 51  | 1     | 2326 | C    |
| 51  | 1     | 2327 | A    |
| 51  | 1     | 2333 | A    |
| 51  | 1     | 2334 | U    |
| 51  | 1     | 2345 | G    |
| 51  | 1     | 2350 | C    |
| 51  | 1     | 2382 | G    |
| 51  | 1     | 2383 | G    |
| 51  | 1     | 2385 | C    |
| 51  | 1     | 2392 | A    |
| 51  | 1     | 2402 | U    |
| 51  | 1     | 2406 | A    |
| 51  | 1     | 2407 | A    |
| 51  | 1     | 2423 | U    |
| 51  | 1     | 2426 | A    |
| 51  | 1     | 2427 | C    |
| 51  | 1     | 2429 | G    |
| 51  | 1     | 2430 | A    |
| 51  | 1     | 2435 | A    |
| 51  | 1     | 2436 | G    |
| 51  | 1     | 2440 | C    |
| 51  | 1     | 2441 | U    |
| 51  | 1     | 2445 | G    |
| 51  | 1     | 2447 | G    |
| 51  | 1     | 2448 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 2476 | A    |
| 51  | 1     | 2482 | A    |
| 51  | 1     | 2491 | U    |
| 51  | 1     | 2492 | U    |
| 51  | 1     | 2498 | C    |
| 51  | 1     | 2502 | G    |
| 51  | 1     | 2505 | G    |
| 51  | 1     | 2506 | U    |
| 51  | 1     | 2507 | C    |
| 51  | 1     | 2518 | A    |
| 51  | 1     | 2547 | A    |
| 51  | 1     | 2554 | U    |
| 51  | 1     | 2566 | A    |
| 51  | 1     | 2567 | G    |
| 51  | 1     | 2572 | A    |
| 51  | 1     | 2573 | C    |
| 51  | 1     | 2582 | G    |
| 51  | 1     | 2602 | A    |
| 51  | 1     | 2609 | U    |
| 51  | 1     | 2613 | U    |
| 51  | 1     | 2629 | U    |
| 51  | 1     | 2630 | G    |
| 51  | 1     | 2642 | G    |
| 51  | 1     | 2646 | C    |
| 51  | 1     | 2689 | U    |
| 51  | 1     | 2690 | U    |
| 51  | 1     | 2714 | G    |
| 51  | 1     | 2726 | A    |
| 51  | 1     | 2732 | G    |
| 51  | 1     | 2744 | G    |
| 51  | 1     | 2748 | A    |
| 51  | 1     | 2751 | G    |
| 51  | 1     | 2758 | A    |
| 51  | 1     | 2764 | A    |
| 51  | 1     | 2765 | A    |
| 51  | 1     | 2778 | A    |
| 51  | 1     | 2779 | U    |
| 51  | 1     | 2793 | C    |
| 51  | 1     | 2798 | U    |
| 51  | 1     | 2799 | A    |
| 51  | 1     | 2800 | A    |
| 51  | 1     | 2801 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 2820 | A    |
| 51  | 1     | 2861 | U    |
| 51  | 1     | 2867 | G    |
| 51  | 1     | 2868 | A    |
| 51  | 1     | 2872 | A    |
| 51  | 1     | 2879 | A    |
| 51  | 1     | 2880 | C    |
| 51  | 1     | 2884 | U    |
| 51  | 1     | 2901 | C    |
| 52  | 2     | 9    | G    |
| 52  | 2     | 13   | G    |
| 52  | 2     | 25   | U    |
| 52  | 2     | 30   | C    |
| 52  | 2     | 35   | C    |
| 52  | 2     | 36   | C    |
| 52  | 2     | 44   | G    |
| 52  | 2     | 45   | A    |
| 52  | 2     | 53   | A    |
| 52  | 2     | 67   | G    |
| 52  | 2     | 87   | U    |
| 52  | 2     | 88   | C    |
| 52  | 2     | 89   | U    |
| 52  | 2     | 90   | C    |
| 52  | 2     | 108  | A    |
| 52  | 2     | 109  | A    |
| 52  | 2     | 120  | A    |
| 53  | 3     | 4    | U    |
| 53  | 3     | 5    | U    |
| 53  | 3     | 6    | G    |
| 53  | 3     | 7    | A    |
| 53  | 3     | 9    | G    |
| 53  | 3     | 22   | G    |
| 53  | 3     | 32   | A    |
| 53  | 3     | 39   | G    |
| 53  | 3     | 47   | C    |
| 53  | 3     | 48   | C    |
| 53  | 3     | 51   | A    |
| 53  | 3     | 71   | A    |
| 53  | 3     | 75   | G    |
| 53  | 3     | 77   | A    |
| 53  | 3     | 78   | A    |
| 53  | 3     | 80   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 3     | 83  | C    |
| 53  | 3     | 84  | U    |
| 53  | 3     | 87  | C    |
| 53  | 3     | 88  | U    |
| 53  | 3     | 94  | G    |
| 53  | 3     | 95  | C    |
| 53  | 3     | 100 | G    |
| 53  | 3     | 108 | G    |
| 53  | 3     | 116 | A    |
| 53  | 3     | 121 | U    |
| 53  | 3     | 127 | G    |
| 53  | 3     | 130 | A    |
| 53  | 3     | 144 | G    |
| 53  | 3     | 163 | C    |
| 53  | 3     | 183 | C    |
| 53  | 3     | 197 | A    |
| 53  | 3     | 206 | C    |
| 53  | 3     | 208 | U    |
| 53  | 3     | 210 | C    |
| 53  | 3     | 211 | G    |
| 53  | 3     | 212 | G    |
| 53  | 3     | 222 | C    |
| 53  | 3     | 226 | G    |
| 53  | 3     | 240 | G    |
| 53  | 3     | 245 | U    |
| 53  | 3     | 247 | G    |
| 53  | 3     | 251 | G    |
| 53  | 3     | 263 | A    |
| 53  | 3     | 264 | C    |
| 53  | 3     | 266 | G    |
| 53  | 3     | 267 | C    |
| 53  | 3     | 279 | A    |
| 53  | 3     | 280 | C    |
| 53  | 3     | 281 | G    |
| 53  | 3     | 289 | G    |
| 53  | 3     | 293 | G    |
| 53  | 3     | 321 | A    |
| 53  | 3     | 328 | C    |
| 53  | 3     | 329 | A    |
| 53  | 3     | 330 | C    |
| 53  | 3     | 345 | C    |
| 53  | 3     | 347 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 3     | 348 | G    |
| 53  | 3     | 352 | C    |
| 53  | 3     | 353 | A    |
| 53  | 3     | 354 | G    |
| 53  | 3     | 363 | A    |
| 53  | 3     | 367 | U    |
| 53  | 3     | 372 | C    |
| 53  | 3     | 374 | A    |
| 53  | 3     | 388 | G    |
| 53  | 3     | 397 | A    |
| 53  | 3     | 398 | U    |
| 53  | 3     | 405 | U    |
| 53  | 3     | 406 | G    |
| 53  | 3     | 412 | A    |
| 53  | 3     | 413 | G    |
| 53  | 3     | 422 | C    |
| 53  | 3     | 423 | G    |
| 53  | 3     | 428 | G    |
| 53  | 3     | 429 | U    |
| 53  | 3     | 446 | G    |
| 53  | 3     | 453 | G    |
| 53  | 3     | 467 | U    |
| 53  | 3     | 468 | A    |
| 53  | 3     | 472 | U    |
| 53  | 3     | 479 | U    |
| 53  | 3     | 480 | U    |
| 53  | 3     | 481 | G    |
| 53  | 3     | 484 | G    |
| 53  | 3     | 485 | U    |
| 53  | 3     | 486 | U    |
| 53  | 3     | 487 | A    |
| 53  | 3     | 496 | A    |
| 53  | 3     | 497 | G    |
| 53  | 3     | 505 | G    |
| 53  | 3     | 508 | U    |
| 53  | 3     | 509 | A    |
| 53  | 3     | 511 | C    |
| 53  | 3     | 518 | C    |
| 53  | 3     | 521 | G    |
| 53  | 3     | 522 | C    |
| 53  | 3     | 531 | U    |
| 53  | 3     | 532 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 3     | 533 | A    |
| 53  | 3     | 536 | C    |
| 53  | 3     | 547 | A    |
| 53  | 3     | 561 | U    |
| 53  | 3     | 562 | U    |
| 53  | 3     | 564 | C    |
| 53  | 3     | 566 | G    |
| 53  | 3     | 572 | A    |
| 53  | 3     | 573 | A    |
| 53  | 3     | 575 | G    |
| 53  | 3     | 576 | C    |
| 53  | 3     | 577 | G    |
| 53  | 3     | 607 | A    |
| 53  | 3     | 615 | G    |
| 53  | 3     | 633 | G    |
| 53  | 3     | 639 | G    |
| 53  | 3     | 642 | A    |
| 53  | 3     | 653 | U    |
| 53  | 3     | 655 | A    |
| 53  | 3     | 660 | C    |
| 53  | 3     | 665 | A    |
| 53  | 3     | 682 | G    |
| 53  | 3     | 688 | G    |
| 53  | 3     | 702 | A    |
| 53  | 3     | 703 | G    |
| 53  | 3     | 718 | A    |
| 53  | 3     | 721 | G    |
| 53  | 3     | 723 | U    |
| 53  | 3     | 724 | G    |
| 53  | 3     | 731 | G    |
| 53  | 3     | 734 | G    |
| 53  | 3     | 755 | G    |
| 53  | 3     | 777 | A    |
| 53  | 3     | 793 | U    |
| 53  | 3     | 799 | G    |
| 53  | 3     | 809 | G    |
| 53  | 3     | 815 | A    |
| 53  | 3     | 817 | C    |
| 53  | 3     | 818 | G    |
| 53  | 3     | 819 | A    |
| 53  | 3     | 820 | U    |
| 53  | 3     | 821 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 3     | 829  | G    |
| 53  | 3     | 836  | G    |
| 53  | 3     | 843  | U    |
| 53  | 3     | 844  | G    |
| 53  | 3     | 845  | A    |
| 53  | 3     | 846  | G    |
| 53  | 3     | 849  | G    |
| 53  | 3     | 851  | G    |
| 53  | 3     | 868  | C    |
| 53  | 3     | 902  | G    |
| 53  | 3     | 914  | A    |
| 53  | 3     | 934  | C    |
| 53  | 3     | 935  | A    |
| 53  | 3     | 960  | U    |
| 53  | 3     | 961  | U    |
| 53  | 3     | 966  | G    |
| 53  | 3     | 969  | A    |
| 53  | 3     | 971  | G    |
| 53  | 3     | 975  | A    |
| 53  | 3     | 976  | G    |
| 53  | 3     | 977  | A    |
| 53  | 3     | 991  | U    |
| 53  | 3     | 992  | U    |
| 53  | 3     | 993  | G    |
| 53  | 3     | 1004 | A    |
| 53  | 3     | 1020 | G    |
| 53  | 3     | 1028 | C    |
| 53  | 3     | 1031 | C    |
| 53  | 3     | 1032 | G    |
| 53  | 3     | 1033 | G    |
| 53  | 3     | 1034 | G    |
| 53  | 3     | 1036 | A    |
| 53  | 3     | 1053 | G    |
| 53  | 3     | 1054 | C    |
| 53  | 3     | 1055 | A    |
| 53  | 3     | 1085 | U    |
| 53  | 3     | 1094 | G    |
| 53  | 3     | 1095 | U    |
| 53  | 3     | 1099 | G    |
| 53  | 3     | 1101 | A    |
| 53  | 3     | 1108 | G    |
| 53  | 3     | 1133 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 3     | 1136 | C    |
| 53  | 3     | 1137 | C    |
| 53  | 3     | 1139 | G    |
| 53  | 3     | 1158 | C    |
| 53  | 3     | 1159 | U    |
| 53  | 3     | 1168 | U    |
| 53  | 3     | 1171 | A    |
| 53  | 3     | 1182 | G    |
| 53  | 3     | 1183 | U    |
| 53  | 3     | 1184 | G    |
| 53  | 3     | 1195 | C    |
| 53  | 3     | 1196 | A    |
| 53  | 3     | 1197 | A    |
| 53  | 3     | 1202 | U    |
| 53  | 3     | 1206 | G    |
| 53  | 3     | 1224 | U    |
| 53  | 3     | 1225 | A    |
| 53  | 3     | 1226 | C    |
| 53  | 3     | 1227 | A    |
| 53  | 3     | 1237 | C    |
| 53  | 3     | 1238 | A    |
| 53  | 3     | 1240 | U    |
| 53  | 3     | 1241 | G    |
| 53  | 3     | 1250 | A    |
| 53  | 3     | 1256 | A    |
| 53  | 3     | 1260 | G    |
| 53  | 3     | 1261 | A    |
| 53  | 3     | 1275 | A    |
| 53  | 3     | 1278 | G    |
| 53  | 3     | 1280 | A    |
| 53  | 3     | 1281 | C    |
| 53  | 3     | 1282 | C    |
| 53  | 3     | 1286 | U    |
| 53  | 3     | 1287 | A    |
| 53  | 3     | 1290 | G    |
| 53  | 3     | 1300 | G    |
| 53  | 3     | 1302 | C    |
| 53  | 3     | 1305 | G    |
| 53  | 3     | 1312 | G    |
| 53  | 3     | 1317 | C    |
| 53  | 3     | 1322 | C    |
| 53  | 3     | 1331 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 3     | 1335 | U    |
| 53  | 3     | 1336 | C    |
| 53  | 3     | 1340 | A    |
| 53  | 3     | 1363 | A    |
| 53  | 3     | 1370 | G    |
| 53  | 3     | 1379 | G    |
| 53  | 3     | 1394 | A    |
| 53  | 3     | 1400 | C    |
| 53  | 3     | 1404 | C    |
| 53  | 3     | 1419 | G    |
| 53  | 3     | 1429 | A    |
| 53  | 3     | 1446 | A    |
| 53  | 3     | 1448 | C    |
| 53  | 3     | 1452 | C    |
| 53  | 3     | 1453 | G    |
| 53  | 3     | 1487 | G    |
| 53  | 3     | 1492 | A    |
| 53  | 3     | 1497 | G    |
| 53  | 3     | 1499 | A    |
| 53  | 3     | 1503 | A    |
| 53  | 3     | 1506 | U    |
| 53  | 3     | 1507 | A    |
| 53  | 3     | 1517 | G    |
| 53  | 3     | 1518 | A    |
| 53  | 3     | 1519 | A    |
| 53  | 3     | 1529 | G    |
| 53  | 3     | 1530 | G    |
| 54  | 4     | 2    | U    |
| 54  | 4     | 3    | G    |
| 54  | 4     | 6    | U    |
| 54  | 4     | 7    | C    |
| 54  | 4     | 9    | U    |
| 54  | 4     | 10   | C    |
| 54  | 4     | 11   | U    |
| 54  | 4     | 12   | U    |
| 54  | 4     | 14   | U    |
| 54  | 4     | 15   | U    |
| 54  | 4     | 18   | U    |
| 54  | 4     | 19   | U    |
| 54  | 4     | 20   | U    |
| 54  | 4     | 21   | U    |
| 54  | 4     | 22   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | 4     | 24  | U    |
| 54  | 4     | 25  | U    |
| 54  | 4     | 26  | U    |
| 54  | 4     | 33  | U    |
| 54  | 4     | 34  | U    |
| 54  | 4     | 35  | U    |
| 63  | 5     | 2   | C    |
| 63  | 5     | 7   | A    |
| 63  | 5     | 8   | U    |
| 63  | 5     | 9   | A    |
| 63  | 5     | 11  | C    |
| 63  | 5     | 13  | C    |
| 63  | 5     | 15  | G    |
| 63  | 5     | 17  | C    |
| 63  | 5     | 18  | G    |
| 63  | 5     | 19  | G    |
| 63  | 5     | 20  | U    |
| 63  | 5     | 21  | A    |
| 63  | 5     | 26  | A    |
| 63  | 5     | 28  | G    |
| 63  | 5     | 29  | G    |
| 63  | 5     | 30  | G    |
| 63  | 5     | 32  | U    |
| 63  | 5     | 33  | U    |
| 63  | 5     | 34  | G    |
| 63  | 5     | 36  | A    |
| 63  | 5     | 37  | A    |
| 63  | 5     | 39  | U    |
| 63  | 5     | 40  | C    |
| 63  | 5     | 43  | C    |
| 63  | 5     | 44  | G    |
| 63  | 5     | 46  | G    |
| 63  | 5     | 47  | U    |
| 63  | 5     | 48  | C    |
| 63  | 5     | 49  | C    |
| 63  | 5     | 52  | G    |
| 63  | 5     | 57  | G    |
| 63  | 5     | 58  | A    |
| 63  | 5     | 59  | U    |
| 63  | 5     | 60  | U    |
| 63  | 5     | 61  | C    |
| 63  | 5     | 66  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63  | 5     | 73  | A    |
| 63  | 5     | 74  | C    |
| 63  | 5     | 75  | C    |
| 64  | 6     | 2   | G    |
| 64  | 6     | 7   | G    |
| 64  | 6     | 8   | U    |
| 64  | 6     | 9   | G    |
| 64  | 6     | 19  | G    |
| 64  | 6     | 20  | U    |
| 64  | 6     | 21  | A    |
| 64  | 6     | 22  | G    |
| 64  | 6     | 30  | G    |
| 64  | 6     | 33  | U    |
| 64  | 6     | 34  | C    |
| 64  | 6     | 35  | A    |
| 64  | 6     | 36  | U    |
| 64  | 6     | 42  | G    |
| 64  | 6     | 45  | G    |
| 64  | 6     | 54  | U    |
| 64  | 6     | 55  | U    |
| 64  | 6     | 56  | C    |
| 64  | 6     | 57  | A    |
| 64  | 6     | 64  | G    |
| 64  | 6     | 67  | C    |
| 64  | 6     | 68  | C    |
| 64  | 6     | 70  | G    |
| 64  | 6     | 73  | A    |
| 64  | 6     | 74  | C    |
| 64  | 6     | 75  | C    |
| 64  | 6     | 76  | A    |

All (31) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 481  | G    |
| 51  | 1     | 490  | C    |
| 51  | 1     | 685  | A    |
| 51  | 1     | 764  | A    |
| 51  | 1     | 784  | G    |
| 51  | 1     | 827  | U    |
| 51  | 1     | 859  | G    |
| 51  | 1     | 1020 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 1130 | U    |
| 51  | 1     | 1715 | G    |
| 51  | 1     | 1783 | A    |
| 51  | 1     | 1801 | A    |
| 51  | 1     | 1930 | G    |
| 51  | 1     | 2275 | C    |
| 51  | 1     | 2326 | C    |
| 51  | 1     | 2732 | G    |
| 52  | 2     | 88   | C    |
| 53  | 3     | 4    | U    |
| 53  | 3     | 1035 | A    |
| 53  | 3     | 1139 | G    |
| 53  | 3     | 1224 | U    |
| 54  | 4     | 14   | U    |
| 54  | 4     | 19   | U    |
| 63  | 5     | 7    | A    |
| 63  | 5     | 32   | U    |
| 63  | 5     | 39   | U    |
| 63  | 5     | 48   | C    |
| 63  | 5     | 57   | G    |
| 63  | 5     | 60   | U    |
| 64  | 6     | 33   | U    |
| 64  | 6     | 56   | C    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 68  | GDP  | 0     | 801 | -    | 29,30,30     | 1.14 | 3 (10%)     | 45,47,47    | 1.81 | 8 (17%)     |
| 67  | FUA  | 0     | 800 | -    | 39,40,40     | 1.71 | 3 (7%)      | 50,64,64    | 1.13 | 4 (8%)      |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 68  | GDP  | 0     | 801 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 67  | FUA  | 0     | 800 | -    | -       | 9/16/92/92 | 0/4/4/4 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 67  | 0     | 800 | FUA  | C29-C22 | -9.76 | 1.34        | 1.47     |
| 68  | 0     | 801 | GDP  | C5-C4   | 2.99  | 1.46        | 1.38     |
| 67  | 0     | 800 | FUA  | O5-C29  | -2.63 | 1.23        | 1.30     |
| 68  | 0     | 801 | GDP  | C6-N1   | -2.36 | 1.34        | 1.38     |
| 67  | 0     | 800 | FUA  | C9-C11  | 2.34  | 1.57        | 1.54     |
| 68  | 0     | 801 | GDP  | C4-N9   | -2.08 | 1.32        | 1.38     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 68  | 0     | 801 | GDP  | C5-C4-N3    | -5.78 | 119.19      | 128.39   |
| 68  | 0     | 801 | GDP  | C2-N3-C4    | 5.03  | 120.97      | 112.30   |
| 68  | 0     | 801 | GDP  | N9-C4-N3    | 4.06  | 134.07      | 125.95   |
| 68  | 0     | 801 | GDP  | C6-C5-N7    | 3.66  | 136.94      | 130.29   |
| 67  | 0     | 800 | FUA  | C14-C8-C9   | -2.78 | 104.42      | 109.30   |
| 68  | 0     | 801 | GDP  | C4-C5-N7    | -2.64 | 106.49      | 110.67   |
| 68  | 0     | 801 | GDP  | O6-C6-C5    | -2.40 | 120.20      | 126.53   |
| 67  | 0     | 800 | FUA  | C8-C9-C10   | 2.33  | 118.92      | 116.42   |
| 67  | 0     | 800 | FUA  | C1-C10-C9   | 2.14  | 113.96      | 109.16   |
| 68  | 0     | 801 | GDP  | C5-C6-N1    | 2.07  | 118.52      | 113.25   |
| 68  | 0     | 801 | GDP  | C3'-C2'-C1' | 2.04  | 105.33      | 101.46   |
| 67  | 0     | 800 | FUA  | O1-C11-C9   | 2.03  | 116.49      | 111.11   |

There are no chirality outliers.

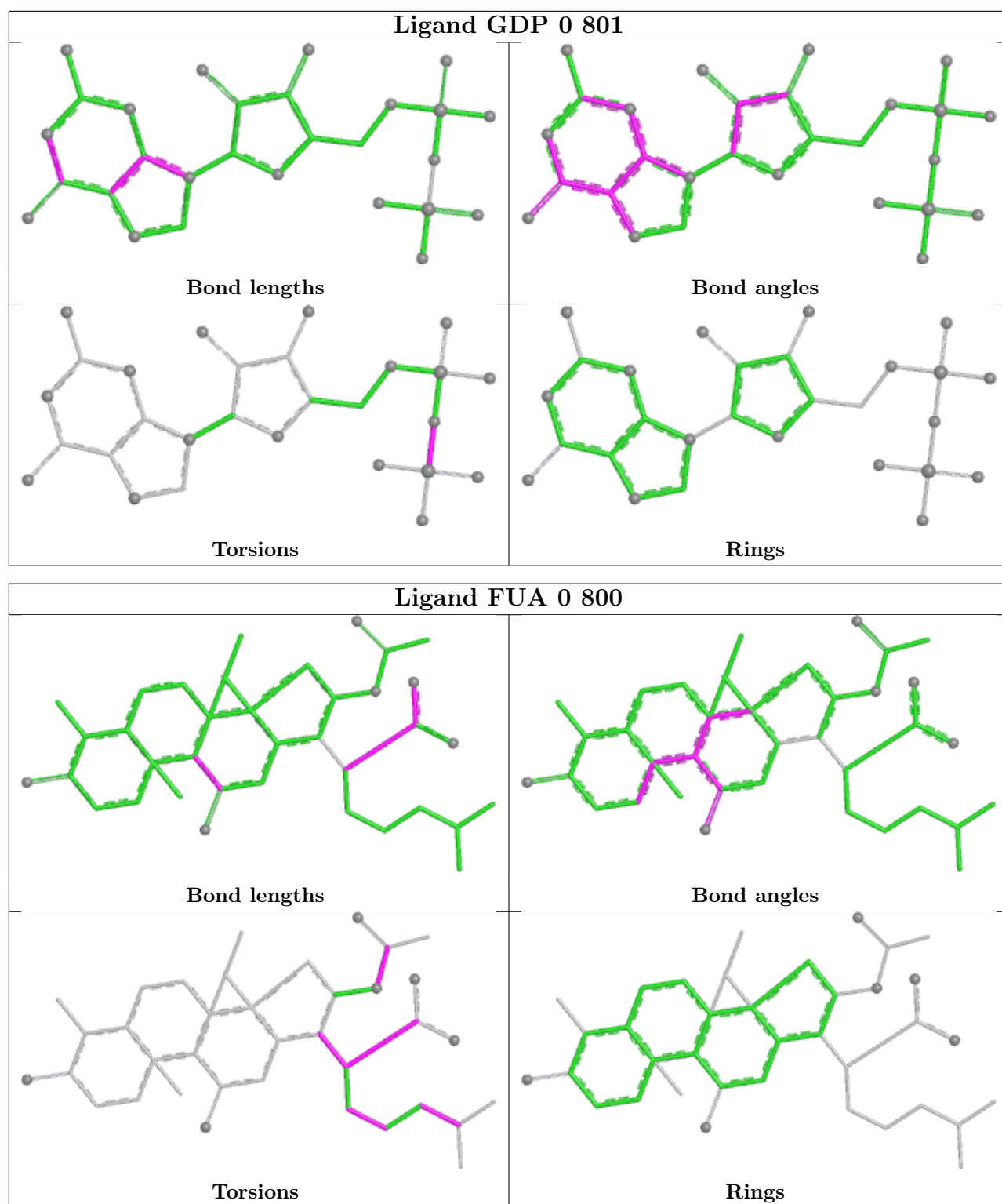
All (11) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 67  | 0     | 800 | FUA  | C13-C17-C22-C23 |
| 67  | 0     | 800 | FUA  | C13-C17-C22-C29 |
| 67  | 0     | 800 | FUA  | C23-C22-C29-O4  |
| 67  | 0     | 800 | FUA  | C23-C22-C29-O5  |
| 67  | 0     | 800 | FUA  | C24-C25-C26-C27 |
| 67  | 0     | 800 | FUA  | C24-C25-C26-C28 |
| 67  | 0     | 800 | FUA  | C32-C31-O2-C16  |
| 68  | 0     | 801 | GDP  | PA-O3A-PB-O2B   |
| 67  | 0     | 800 | FUA  | O3-C31-O2-C16   |
| 67  | 0     | 800 | FUA  | C22-C23-C24-C25 |
| 68  | 0     | 801 | GDP  | PA-O3A-PB-O1B   |

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

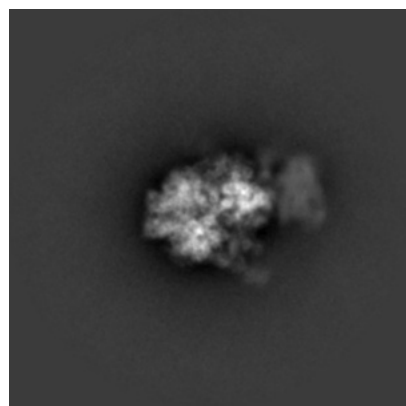
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38947. These allow visual inspection of the internal detail of the map and identification of artifacts.

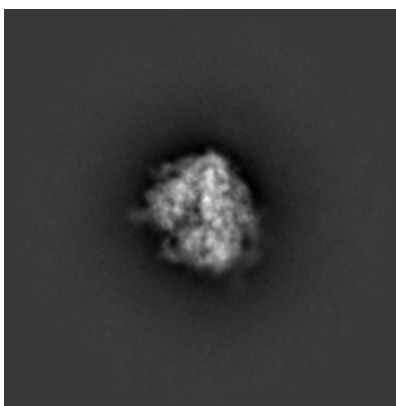
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

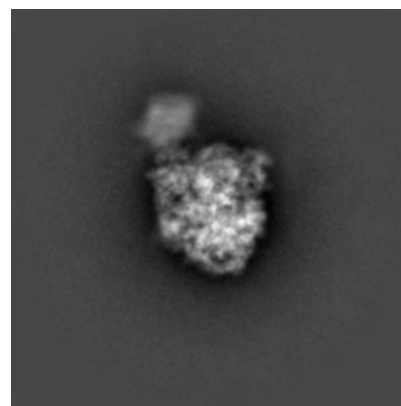
#### 6.1.1 Primary map



X

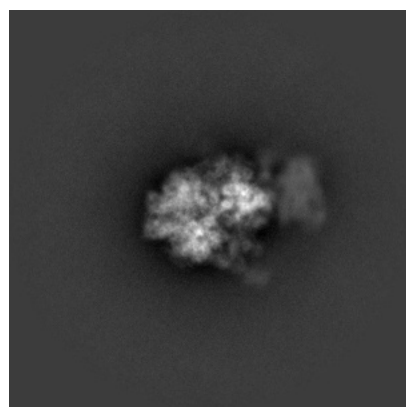


Y

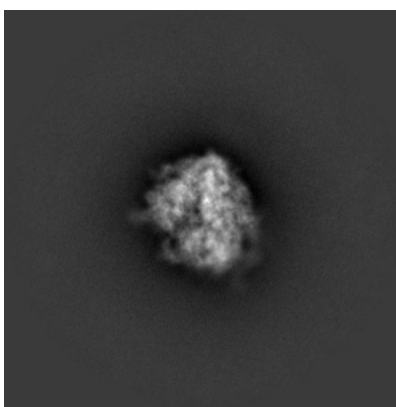


Z

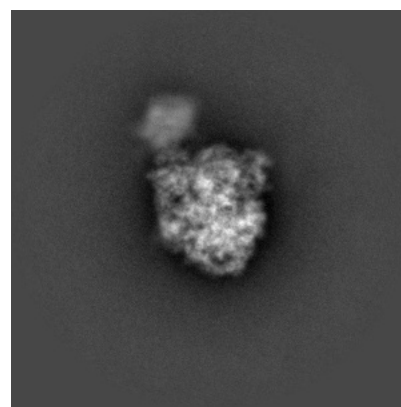
#### 6.1.2 Raw map



X



Y

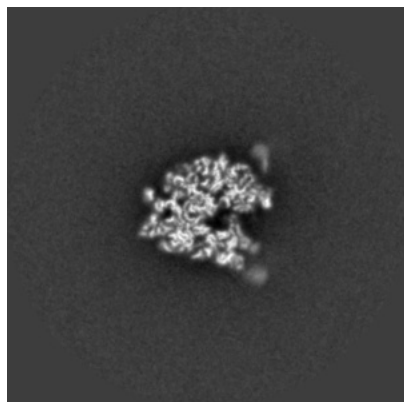


Z

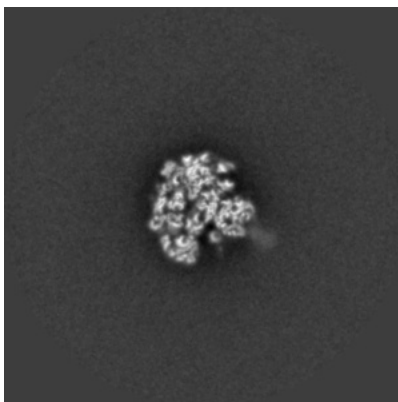
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

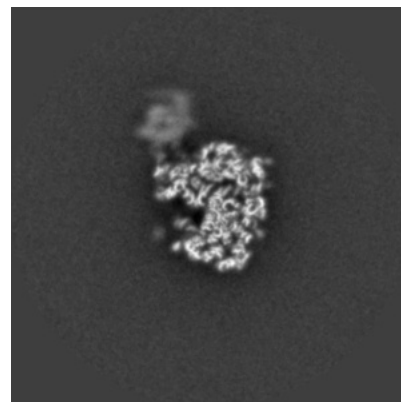
### 6.2.1 Primary map



X Index: 240

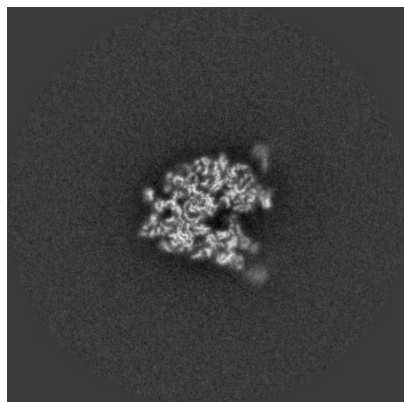


Y Index: 240

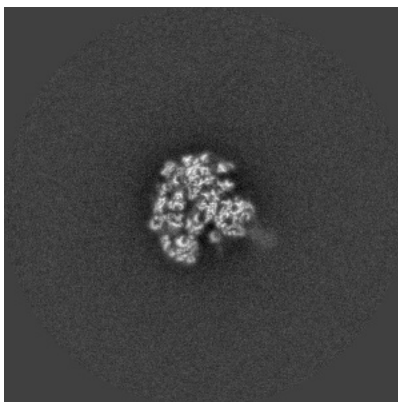


Z Index: 240

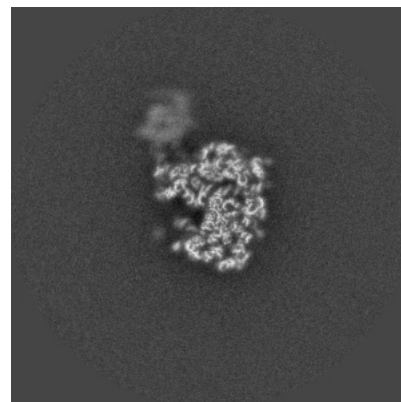
### 6.2.2 Raw map



X Index: 240



Y Index: 240



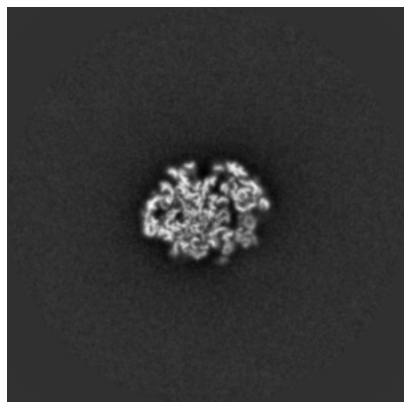
Z Index: 240

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

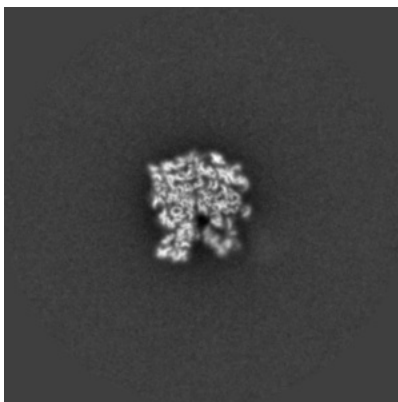


## 6.3 Largest variance slices [i](#)

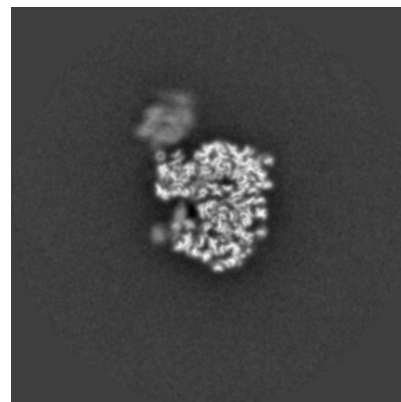
### 6.3.1 Primary map



X Index: 265

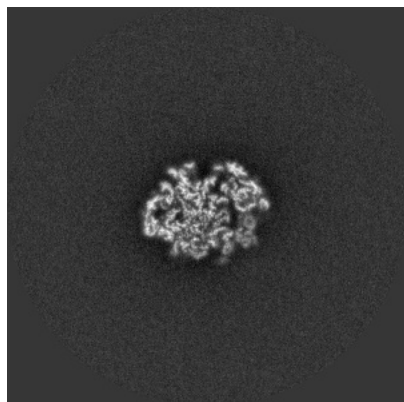


Y Index: 224

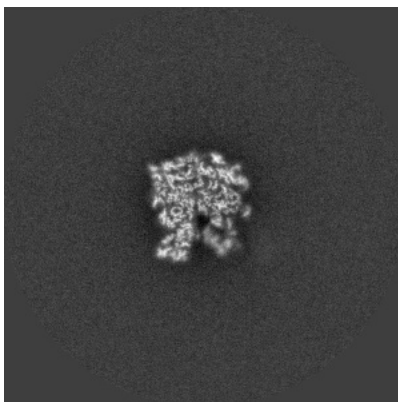


Z Index: 246

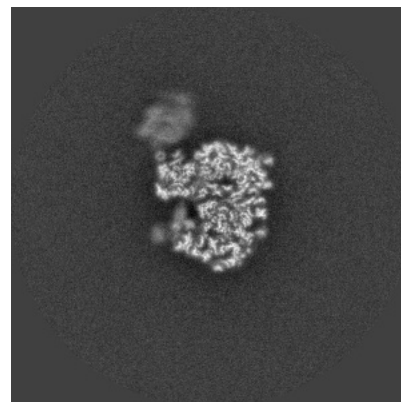
### 6.3.2 Raw map



X Index: 265



Y Index: 224

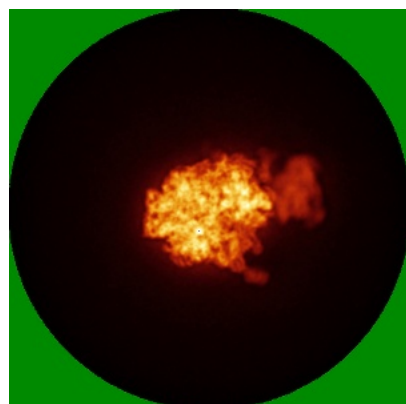


Z Index: 246

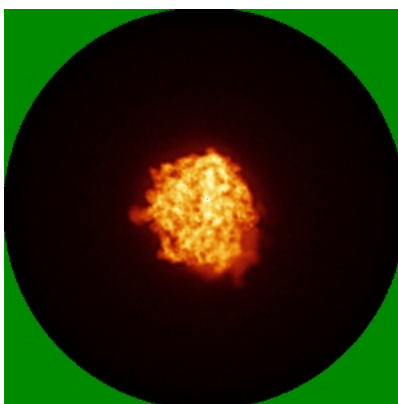
The images above show the largest variance slices of the map in three orthogonal directions.

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

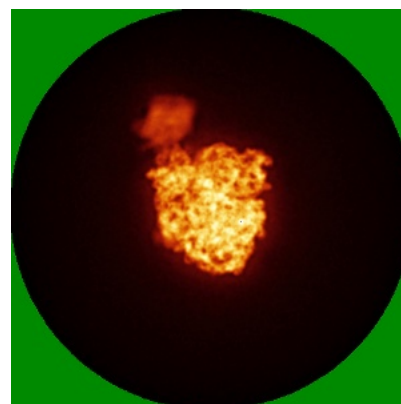
### 6.4.1 Primary map



X

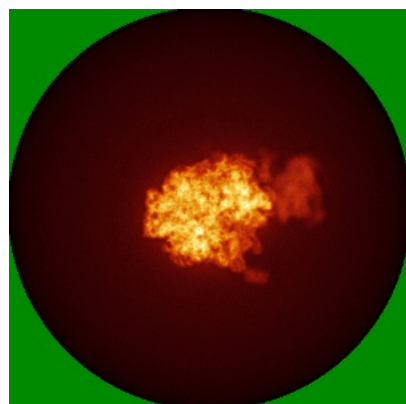


Y

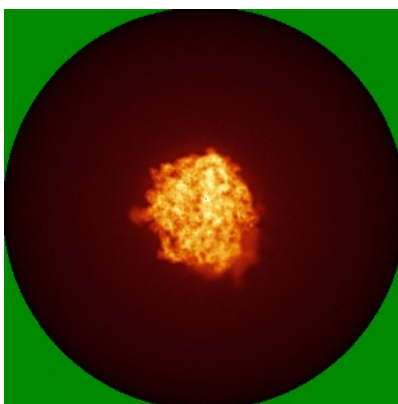


Z

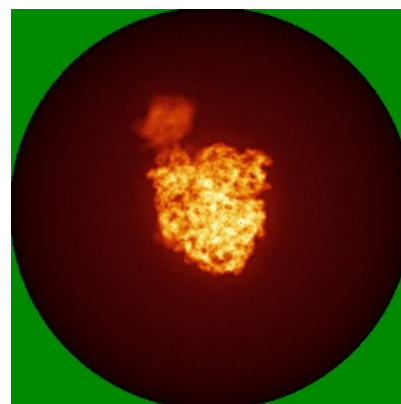
### 6.4.2 Raw map



X



Y



Z

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

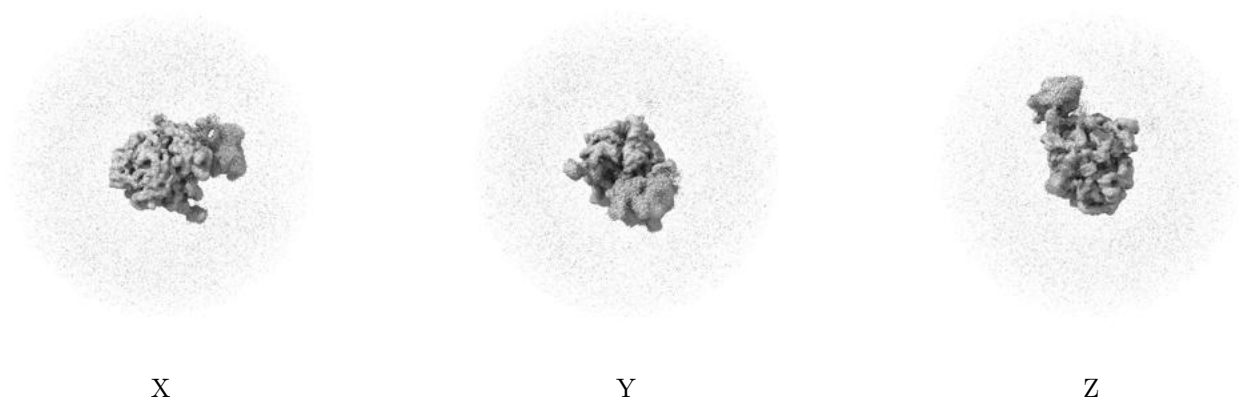
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

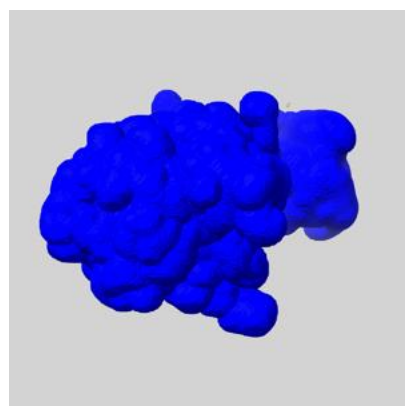
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

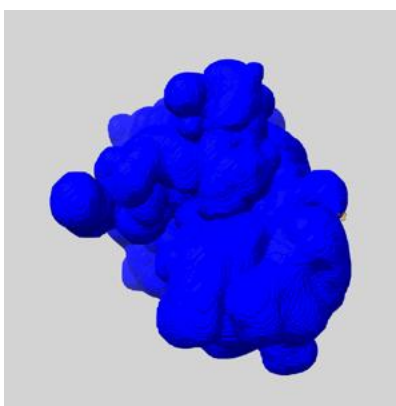
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

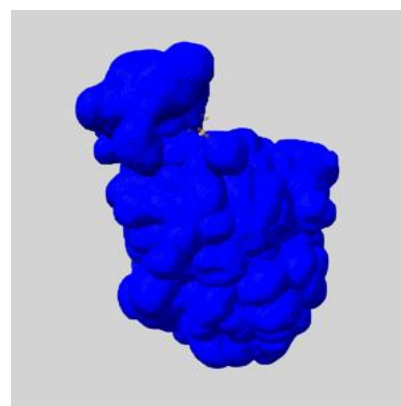
### 6.6.1 emd\_38947\_msk\_1.map [i](#)



X



Y

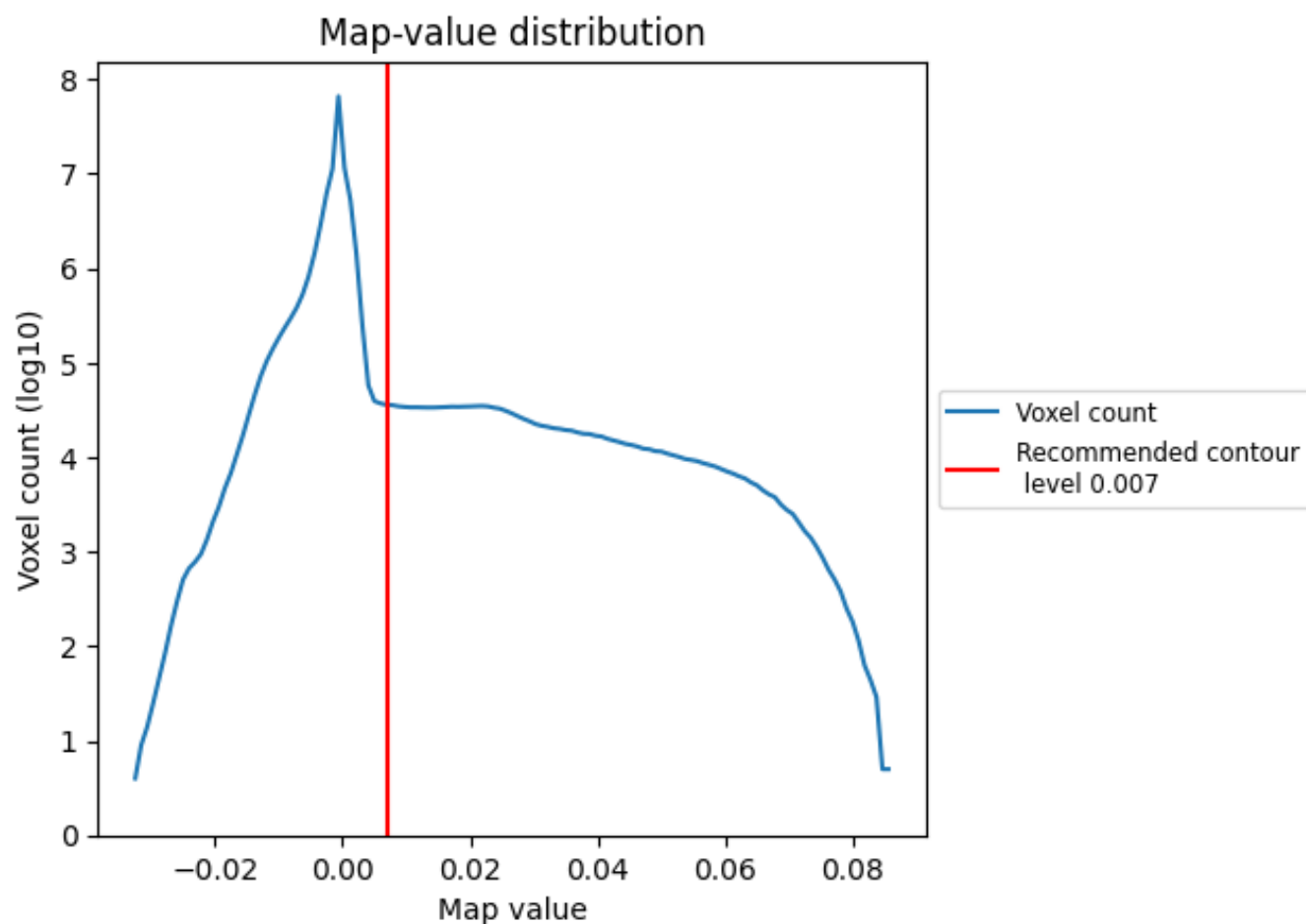


Z

## 7 Map analysis [i](#)

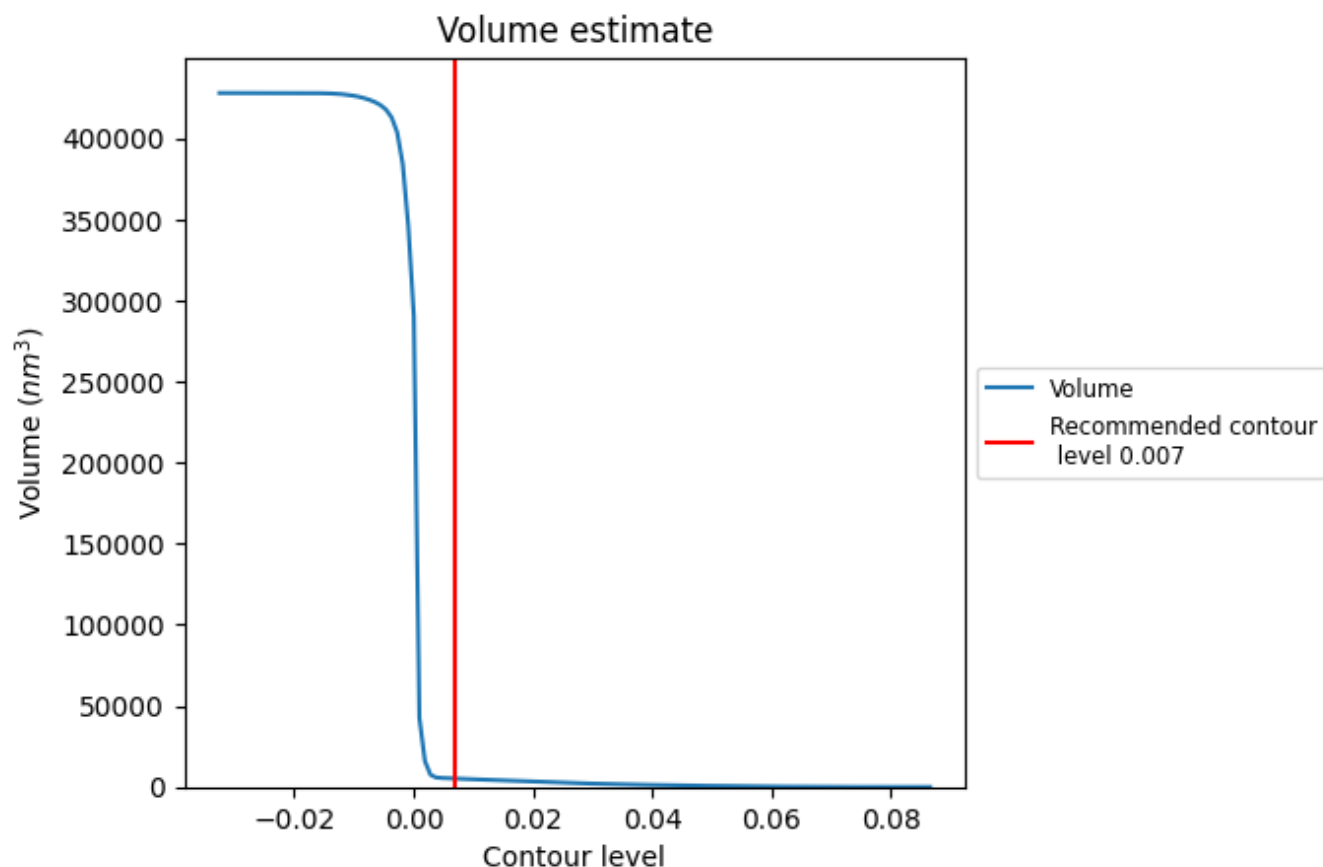
This section contains the results of statistical analysis of the map.

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



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

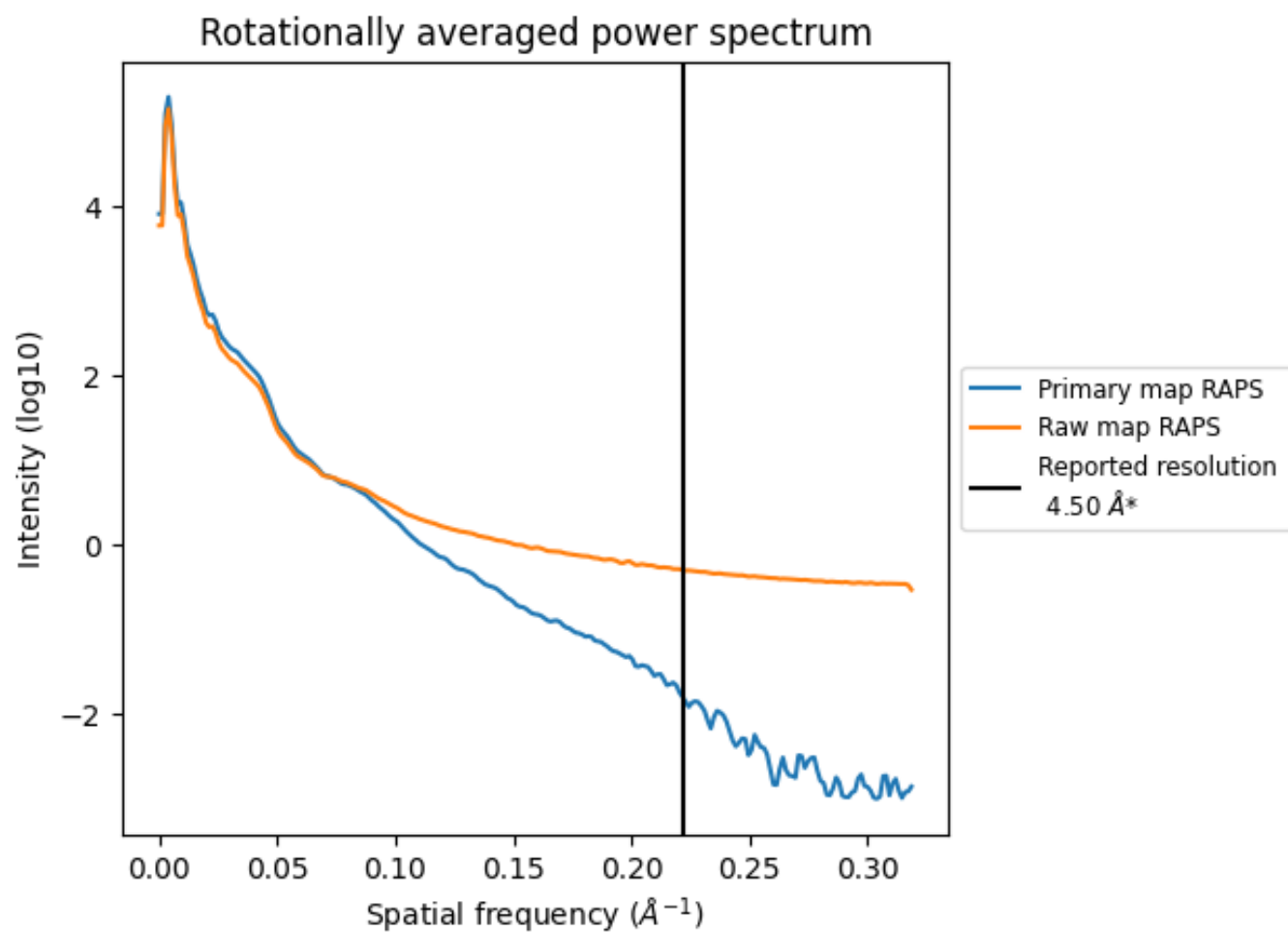
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5179  $\text{nm}^3$ ; this corresponds to an approximate mass of 4678 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

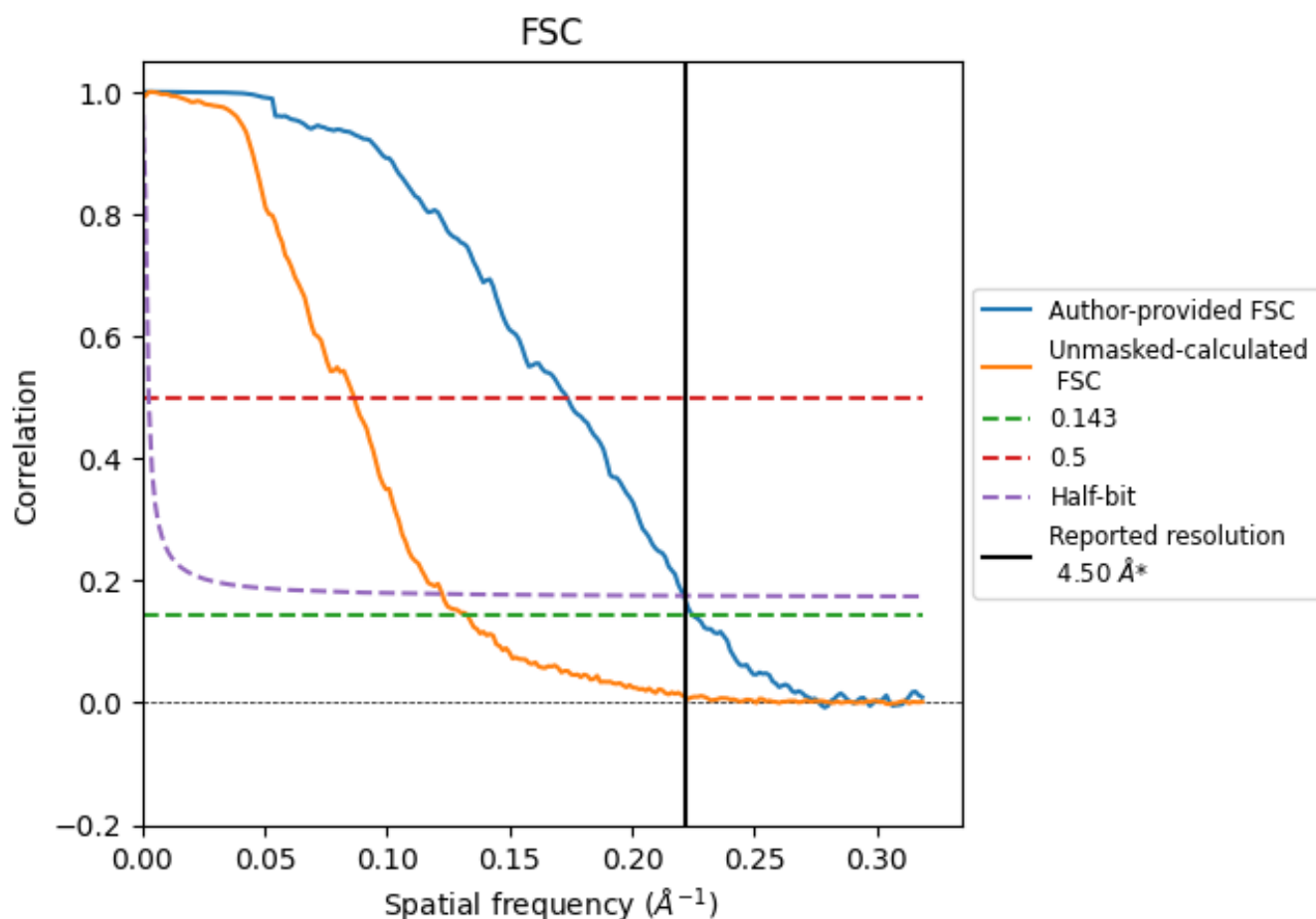


\*Reported resolution corresponds to spatial frequency of 0.222 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.222  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

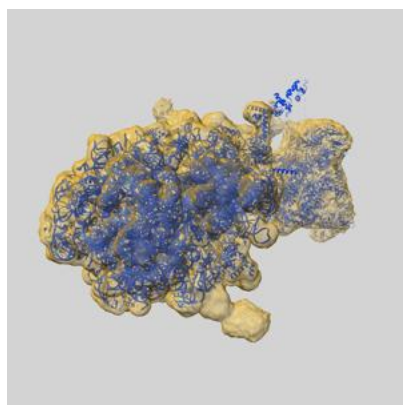
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 4.50                               | -     | -        |
| Author-provided FSC curve | 4.45                               | 5.77  | 4.52     |
| Unmasked-calculated*      | 7.53                               | 11.57 | 8.16     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.53 differs from the reported value 4.5 by more than 10 %

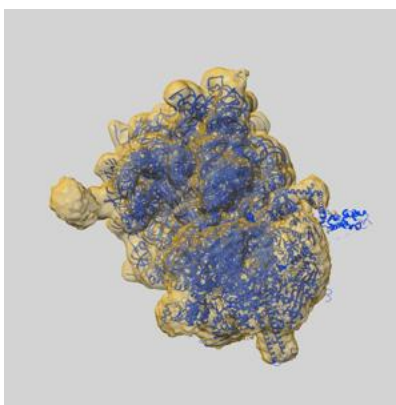
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38947 and PDB model 8Y5R. Per-residue inclusion information can be found in section [3](#) on page [18](#).

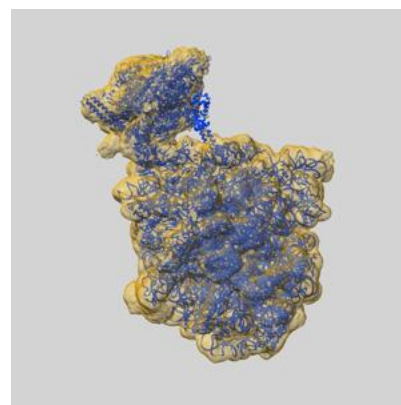
### 9.1 Map-model overlay [i](#)



X



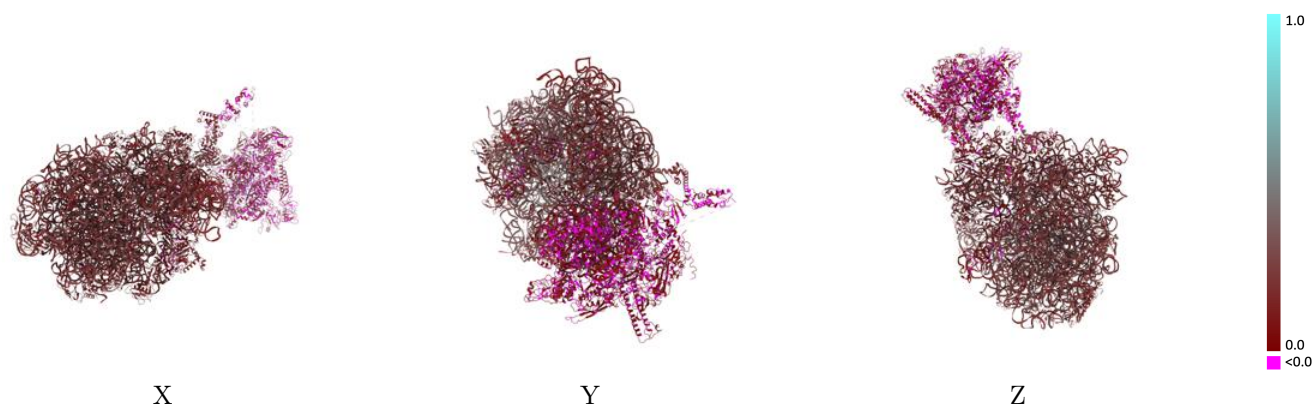
Y



Z

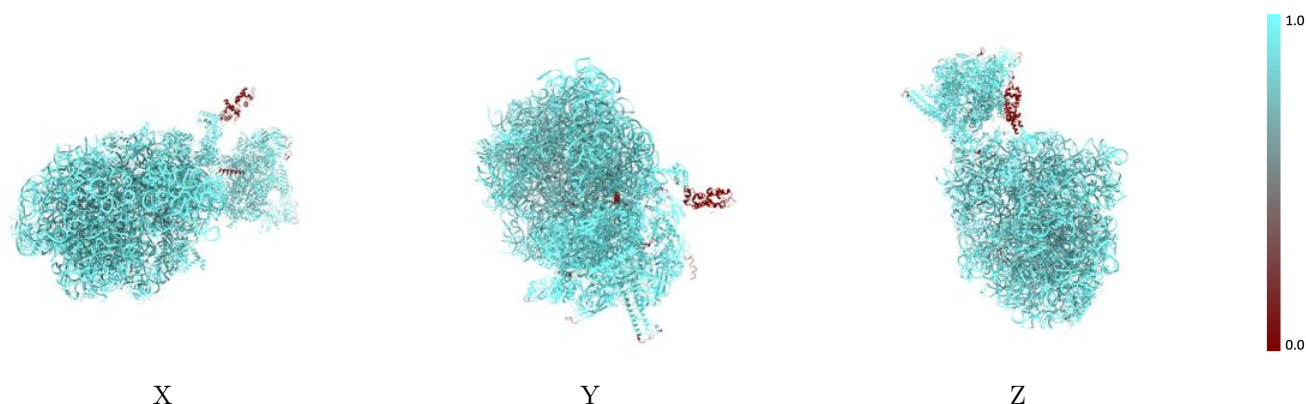
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



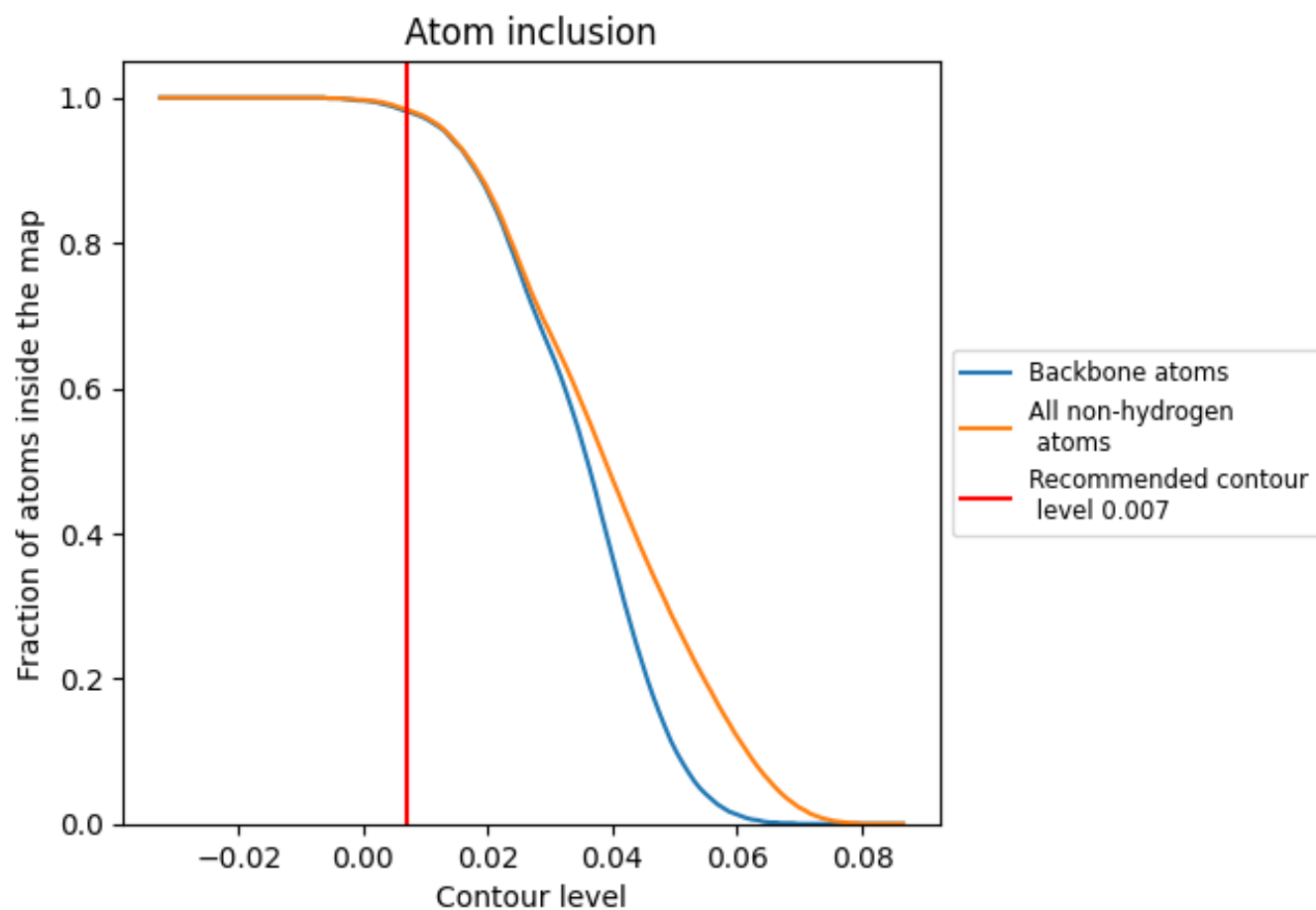
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9840   |  0.1860   |
| 0     |  0.9620   |  0.1590   |
| 1     |  0.9990   |  0.2370   |
| 2     |  1.0000   |  0.2190   |
| 3     |  0.9990   |  0.2220   |
| 4     |  0.9600   |  0.0710   |
| 5     |  0.9770   |  0.1390   |
| 6     |  0.8350   |  0.0860   |
| 8     |  1.0000   |  0.0480   |
| 9     |  1.0000   |  0.0880   |
| A     |  0.9780   |  0.1340   |
| A1    |  0.9270   |  0.0570   |
| A2    |  0.8330   |  0.0560   |
| B     |  0.9950   |  0.1950   |
| B1    |  0.9580  |  0.0460  |
| B2    |  0.9760 |  0.0550 |
| C     |  0.9850 |  0.1850 |
| D     |  0.9860 |  0.1780 |
| E     |  1.0000 |  0.1740 |
| F     |  1.0000 |  0.1580 |
| G     |  0.9900 |  0.1840 |
| H     |  0.9780 |  0.1770 |
| I     |  0.9980 |  0.1480 |
| J     |  0.9930 |  0.1970 |
| K     |  0.9940 |  0.1890 |
| L     |  0.9940 |  0.1930 |
| M     |  0.9850 |  0.1870 |
| N     |  0.9990 |  0.1660 |
| NA    |  0.8350 |  0.1560 |
| NG    |  0.9140 |  0.0750 |
| O     |  1.0000 |  0.1410 |
| P     |  0.9980 |  0.2010 |
| Q     |  0.9460 |  0.1560 |
| R     |  0.9990 |  0.1670 |
| S     |  0.9970 |  0.1300 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| T     |  0.9940   |  0.1650   |
| U     |  0.9980   |  0.1540   |
| V     |  0.9870   |  0.1840   |
| W     |  0.9980   |  0.1550   |
| W0    |  0.5610   |  0.0450   |
| X     |  0.9870   |  0.1100   |
| Y     |  0.9950   |  0.1780   |
| Z     |  0.9770   |  0.1500   |
| b     |  0.9950   |  0.2210   |
| c     |  0.9950   |  0.1920   |
| d     |  0.9960   |  0.1930   |
| e     |  0.9910   |  0.1700   |
| f     |  0.9780   |  0.1860   |
| g     |  0.9980   |  0.1820   |
| i     |  0.9560   |  0.0900   |
| j     |  0.9960   |  0.1930   |
| k     |  0.9880   |  0.2310   |
| l     |  1.0000   |  0.1900   |
| m     |  0.9880   |  0.2080   |
| n     |  1.0000  |  0.1840  |
| o     |  1.0000 |  0.1720 |
| p     |  0.9870 |  0.2130 |
| q     |  0.9990 |  0.1670 |
| r     |  0.9960 |  0.1940 |
| s     |  0.9920 |  0.1970 |
| t     |  0.9890 |  0.1840 |
| u     |  0.9950 |  0.1700 |
| v     |  0.9970 |  0.1800 |
| w     |  1.0000 |  0.1690 |
| x     |  1.0000 |  0.1940 |
| y     |  1.0000 |  0.1660 |
| z     |  0.9950 |  0.1960 |