



## Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 01:17 PM EDT

PDB ID : 5KCS / pdb\_00005kcs  
EMDB ID : EMD-8238  
Title : Cryo-EM structure of the Escherichia coli 70S ribosome in complex with antibiotic Evernimycin, mRNA, TetM and P-site tRNA at 3.9Å resolution  
Authors : Arenz, S.; Juetten, M.F.; Graf, M.; Nguyen, F.; Huter, P.; Polikanov, Y.S.; Blanchard, S.C.; Wilson, D.N.  
Deposited on : 2016-06-06  
Resolution : 3.90 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

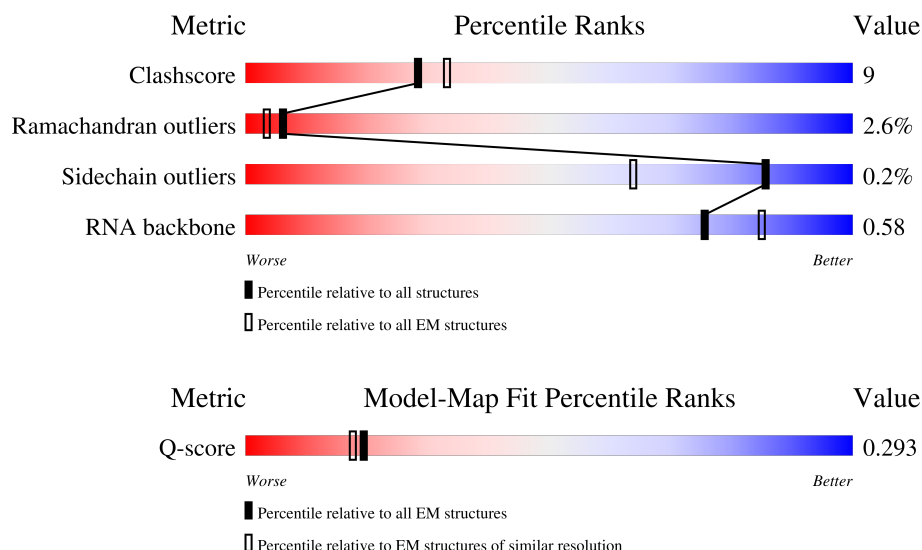
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | 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                       | 8855 ( 3.40 - 4.40 )                                     |

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   | 1A    | 2904   | <div> <div>9%</div> <div>54%</div> <div>39%</div> <div>7%</div> </div> |
| 2   | 1B    | 120    | <div> <div>8%</div> <div>65%</div> <div>29%</div> <div>6%</div> </div> |
| 3   | 1D    | 273    | <div> <div>15%</div> <div>65%</div> <div>34%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | 1E    | 209    |                  |
| 5   | 1F    | 201    |                  |
| 6   | 1G    | 179    |                  |
| 7   | 1H    | 177    |                  |
| 8   | 1L    | 121    |                  |
| 9   | 1I    | 149    |                  |
| 10  | 1J    | 165    |                  |
| 11  | 1K    | 142    |                  |
| 12  | 1N    | 142    |                  |
| 13  | 1O    | 123    |                  |
| 14  | 1P    | 144    |                  |
| 15  | 1Q    | 136    |                  |
| 16  | 1R    | 127    |                  |
| 17  | 1S    | 117    |                  |
| 18  | 1T    | 115    |                  |
| 19  | 1U    | 118    |                  |
| 20  | 1V    | 103    |                  |
| 21  | 1W    | 110    |                  |
| 22  | 1X    | 100    |                  |
| 23  | 1Y    | 104    |                  |
| 24  | 1Z    | 94     |                  |
| 25  | 10    | 85     |                  |
| 26  | 11    | 78     |                  |
| 27  | 12    | 63     |                  |
| 28  | 13    | 59     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | 14    | 70     |                  |
| 30  | 15    | 57     |                  |
| 31  | 16    | 55     |                  |
| 32  | 17    | 46     |                  |
| 33  | 18    | 65     |                  |
| 34  | 19    | 38     |                  |
| 35  | 1a    | 1539   |                  |
| 36  | 1b    | 241    |                  |
| 37  | 1c    | 233    |                  |
| 38  | 1d    | 206    |                  |
| 39  | 1e    | 167    |                  |
| 40  | 1f    | 135    |                  |
| 41  | 1g    | 179    |                  |
| 42  | 1h    | 130    |                  |
| 43  | 1i    | 130    |                  |
| 44  | 1j    | 103    |                  |
| 45  | 1k    | 129    |                  |
| 46  | 1l    | 124    |                  |
| 47  | 1m    | 118    |                  |
| 48  | 1n    | 101    |                  |
| 49  | 1o    | 89     |                  |
| 50  | 1p    | 82     |                  |
| 51  | 1q    | 84     |                  |
| 52  | 1r    | 75     |                  |
| 53  | 1s    | 92     |                  |

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| Mol | Chain | Length | Quality of chain                                                                                                                       |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------------------------------------|
| 54  | 1t    | 87     | <div><div></div><div>44%</div><div></div><div>74%</div><div></div><div>24%</div><div></div></div>                                      |
| 55  | 1u    | 71     | <div><div></div><div>86%</div><div></div><div>61%</div><div></div><div>28%</div><div></div><div>8%</div></div>                         |
| 56  | 1v    | 60     | <div><div></div><div>7%</div><div></div><div>7%</div><div></div><div>8%</div><div></div><div>85%</div></div>                           |
| 57  | 1w    | 639    | <div><div></div><div>28%</div><div></div><div>95%</div><div></div><div>5%</div></div>                                                  |
| 58  | 1x    | 77     | <div><div></div><div>13%</div><div></div><div>49%</div><div></div><div>40%</div><div></div><div>5%</div><div></div><div>5%</div></div> |

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 148945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1   | 1A    | 2900     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62276 | 27788 | 11459 | 20129 | 2900 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference    |
|-------|---------|----------|--------|----------|--------------|
| 1A    | 1847    | G        | A      | conflict | GB 802133627 |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 2   | 1B    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2570  | 1144 | 468 | 838 | 120 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | 1D    | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | 1E    | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | 1F    | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | 1G    | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | 1H    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L7/L12.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 8   | 1L    | 69       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 276   | 138 | 69 | 69 |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | 1I    | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | 1J    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 988   | 625 | 175 | 183 | 5 |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | 1K    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | 1N    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | 1O    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 938   | 587 | 180 | 165 | 6 |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | 1P    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | 1Q    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | 1R    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 17  | 1S    | 116      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | 1T    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 19  | 1U    | 117      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | 1V    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | 1W    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | 1X    | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | 1Y    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |   |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | 1Z    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | 10    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 575   | 356 | 116 | 102 | 1 |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | 11    | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 27  | 12    | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | 13    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29  | 14    | 66       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 522   | 323 | 99 | 94 | 6 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30  | 15    | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 31  | 16    | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 263 | 75 | 71 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32  | 17    | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 33  | 18    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 34  | 19    | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 35 is a RNA chain called 16S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 35  | 1a    | 1539     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33029 | 14738 | 6052 | 10700 | 1539 |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36  | 1b    | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1704  | 1081 | 305 | 311 | 7 |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 37  | 1c    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |       |

- Molecule 38 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38  | 1d    | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 39 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | 1e    | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1141  | 709 | 218 | 208 | 6 |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | 1f    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 817   | 515 | 148 | 148 | 6 |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | 1g    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1181  | 735 | 227 | 215 | 4 |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | 1h    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | 1i    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | 1j    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |       |

- Molecule 45 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | 1k    | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 869   | 535 | 173 | 158 | 3 |         |       |

- Molecule 46 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | 1l    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | 1m    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 883   | 546 | 178 | 156 | 3 |         |       |

- Molecule 48 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | 1n    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 794   | 495 | 164 | 132 | 3 |         |       |

- Molecule 49 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | 1o    | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 50 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | 1p    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 51 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | 1q    | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |       |

- Molecule 52 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 52  | 1r    | 65       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 504   | 317 | 96 | 91 |         |       |

- Molecule 53 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | 1s    | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 637   | 408 | 120 | 107 | 2 |         |       |

- Molecule 54 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | 1t    | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |       |

- Molecule 55 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 55  | 1u    | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 495   | 307 | 100 | 87 | 1 |         |       |

- Molecule 56 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 56  | 1v    | 9        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 192   | 86 | 35 | 62 | 9 |         |       |

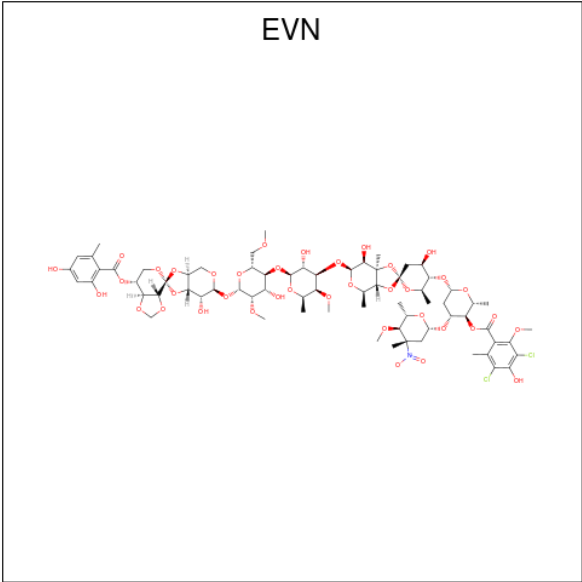
- Molecule 57 is a protein called Tetracycline resistance protein TetM from transposon Tn916.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 57  | 1w    | 639      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2590  | 1308 | 640 | 642 |         |       |

- Molecule 58 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 58  | 1x    | 73       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1567  | 699 | 285 | 510 | 73 |         |       |

- Molecule 59 is (2R,3R,4R,6S)-6-([(2R,3aR,4R,4'R,5'S,6S,6'R,7S,7aR)-6-([(2S,3R,4R,5S,6R)-2-([(2R,3S,4S,5S,6S)-6-([(2R,3aS,3a'R,6S,7R,7' R,7aS,7a'S)-7'-[(2,4-dihydroxy-6-methyl benzoyl)oxy]-7-hydroxyoctahydro-4H-2,4'-spirobi[[1,3]dioxolo[4,5-c]pyran]-6-yl)oxy]-4-hydroxy-5-methoxy-2-(methoxymethyl)tetrahydro-2H-pyran-3-yl)oxy}-3-hydroxy-5-methoxy-6-methyltetrahydro-2H-pyran-4-yl)oxy}-4',7-dihydroxy-4,6',7a-trimethyloctahydro-4H-spiro[1,3-dioxolo[4,5-c]pyran-2,2'-pyran]-5'-yl)oxy}-4-([(2R,4S,5R,6S)-5-methoxy-4,6-dimethyl-4-nitrotetrahydro-2H-pyran-2-yl)oxy]-2-methyltetrahydro-2H-pyran-3-yl 3,5-dichloro-4-hydroxy-2-methoxy-6-methylbenzoate (non-preferred name) (CCD ID: EVN) (formula: C<sub>70</sub>H<sub>97</sub>Cl<sub>2</sub>NO<sub>38</sub>).

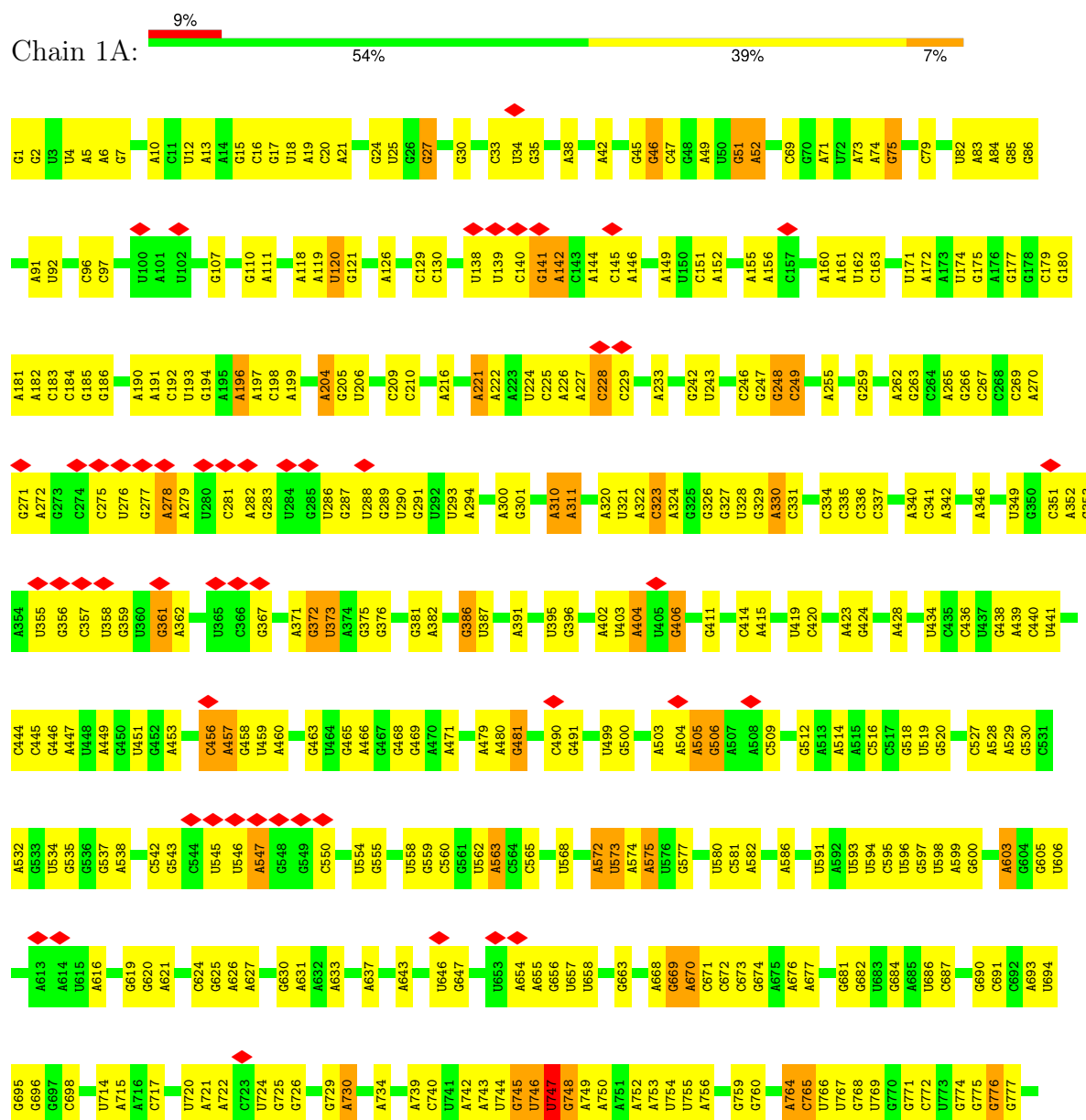


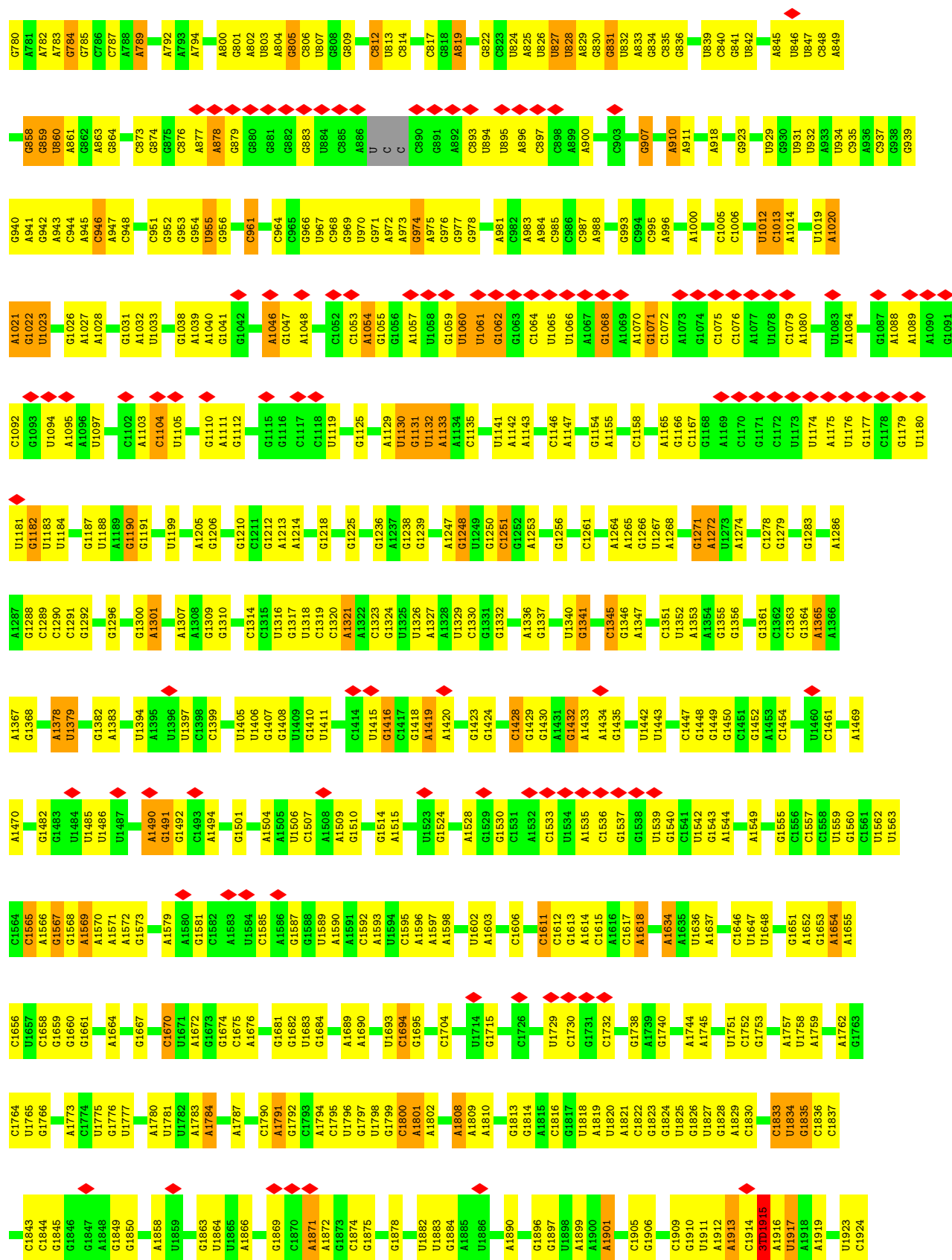
| Mol | Chain | Residues | Atoms |    |    |   |    | AltConf |
|-----|-------|----------|-------|----|----|---|----|---------|
|     |       |          | Total | C  | Cl | N | O  |         |
| 59  | 1A    | 1        | 111   | 70 | 2  | 1 | 38 | 0       |

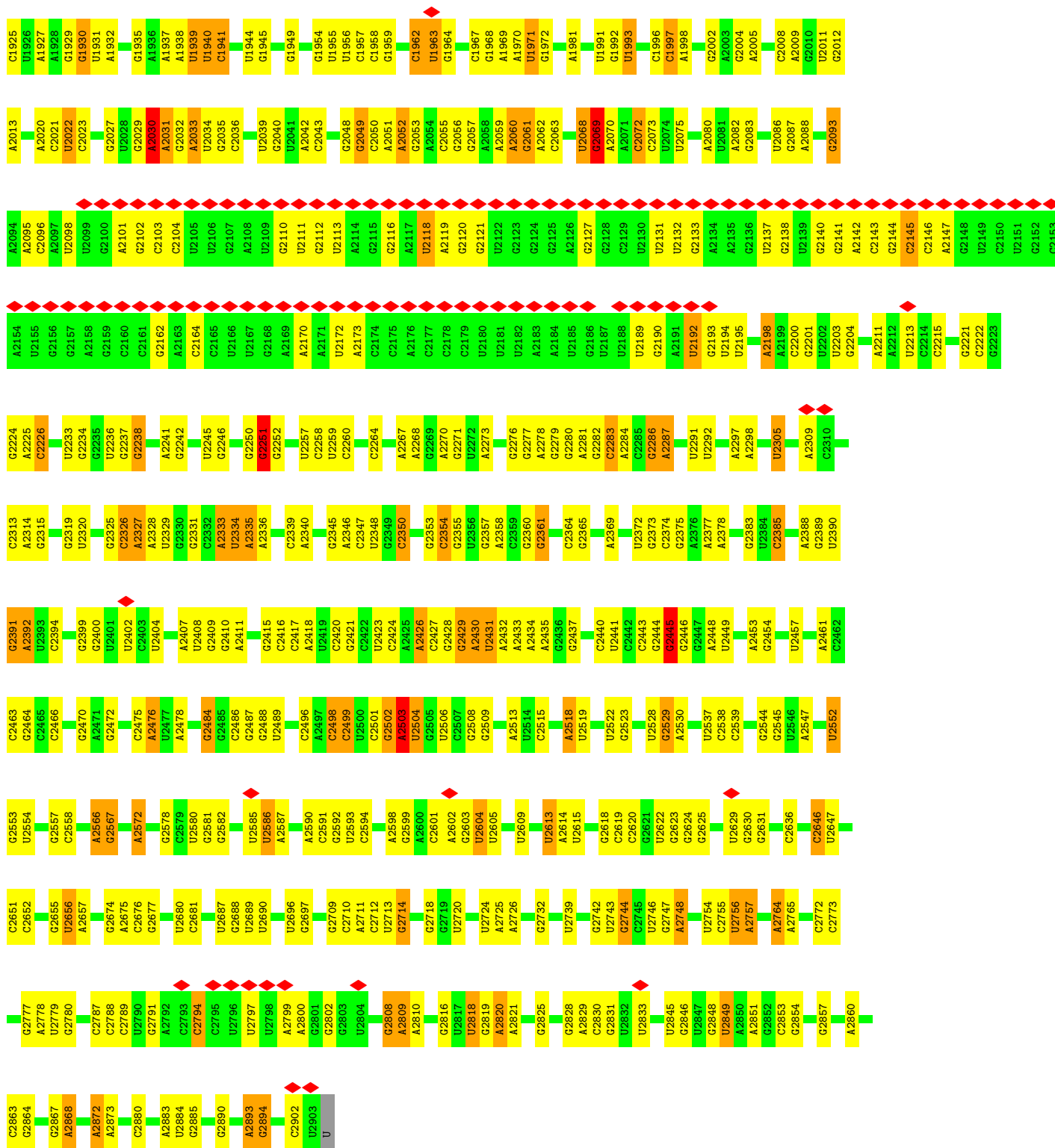
### 3 Residue-property plots

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

#### • Molecule 1: 23S Ribosomal RNA

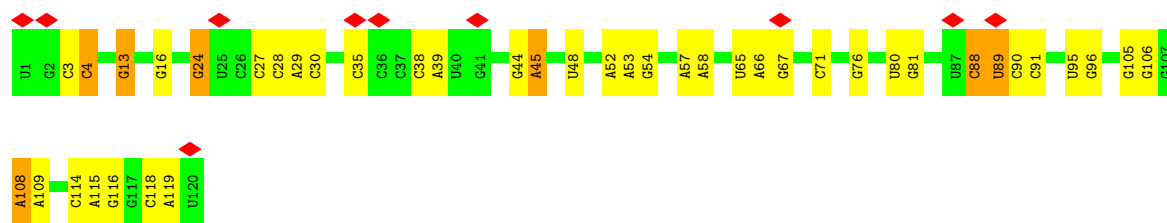




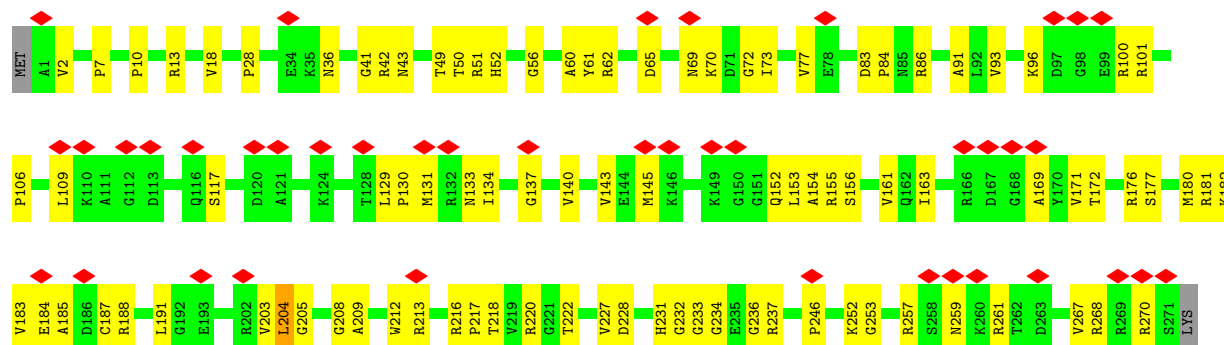


• Molecule 2: 5S Ribosomal RNA

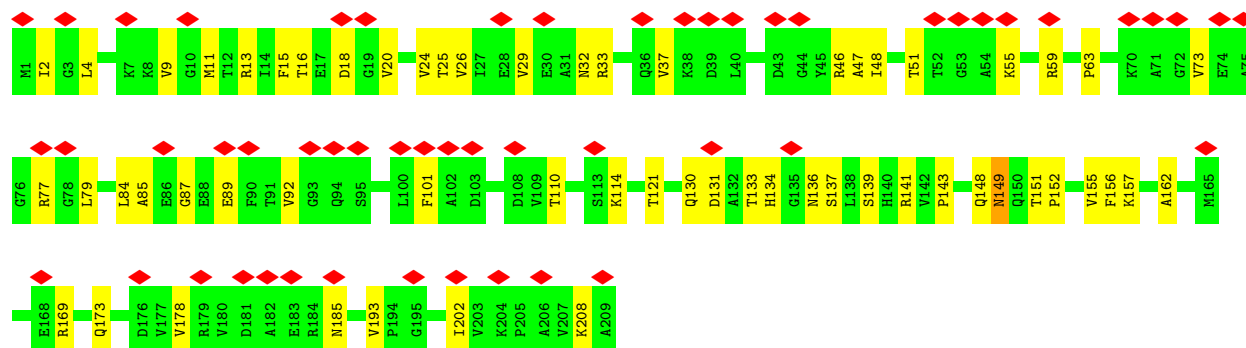
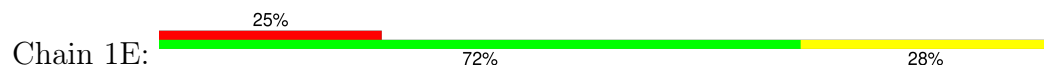




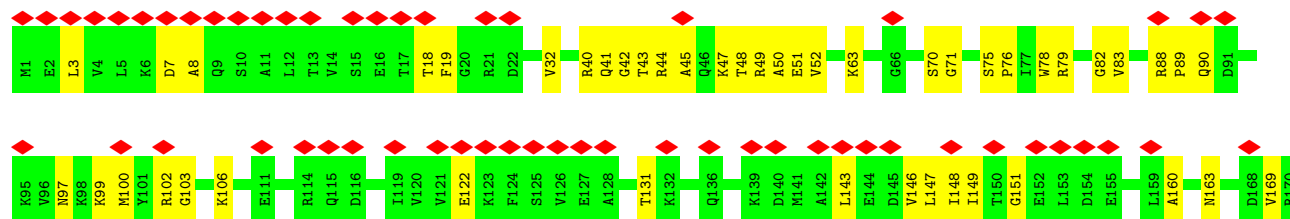
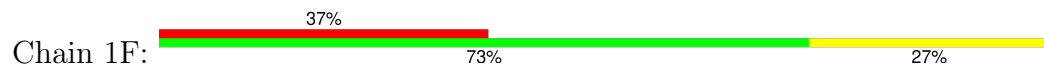
• Molecule 3: 50S ribosomal protein L2

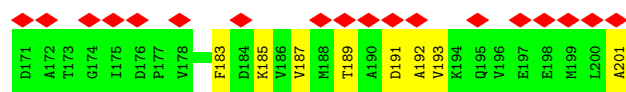


• Molecule 4: 50S ribosomal protein L3



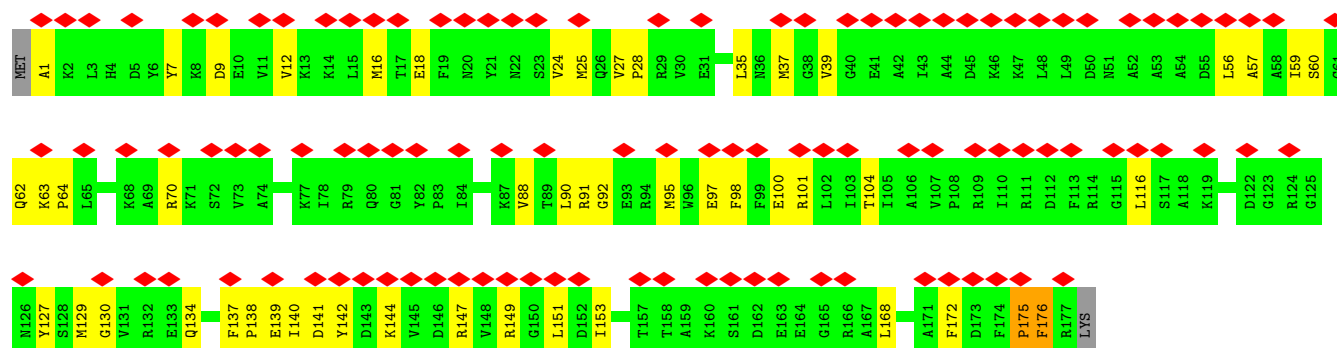
• Molecule 5: 50S ribosomal protein L4





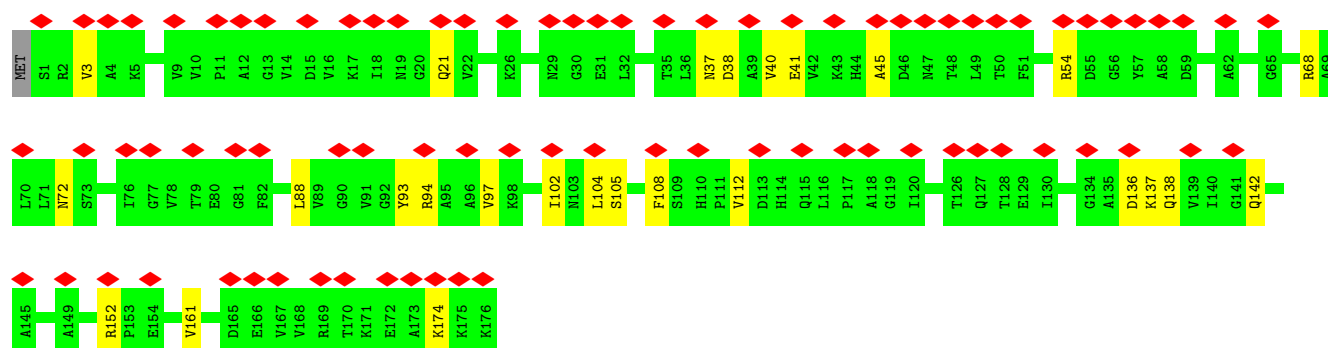
- Molecule 6: 50S ribosomal protein L5

Chain 1G: 61% 70% 27% ..



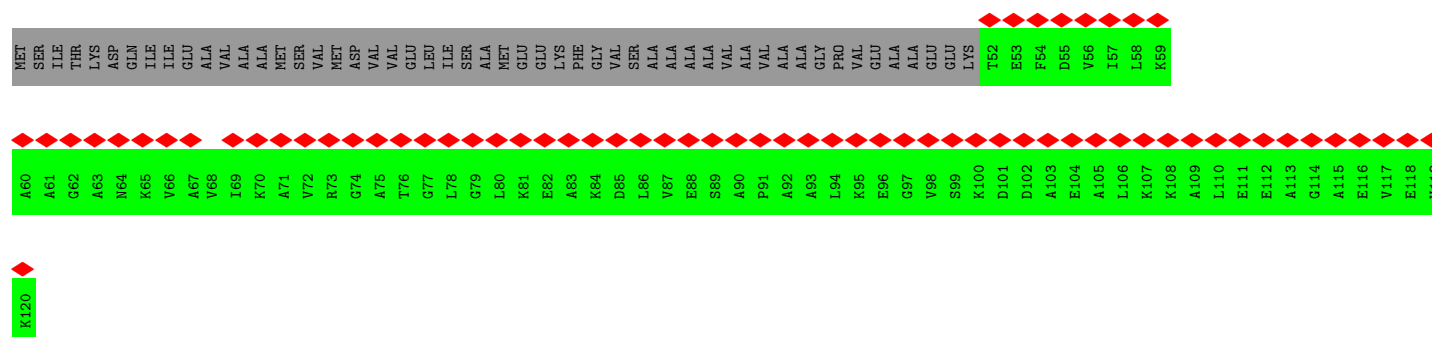
- Molecule 7: 50S ribosomal protein L6

Chain 1H: 46% 85% 15% .

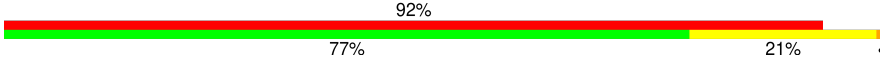


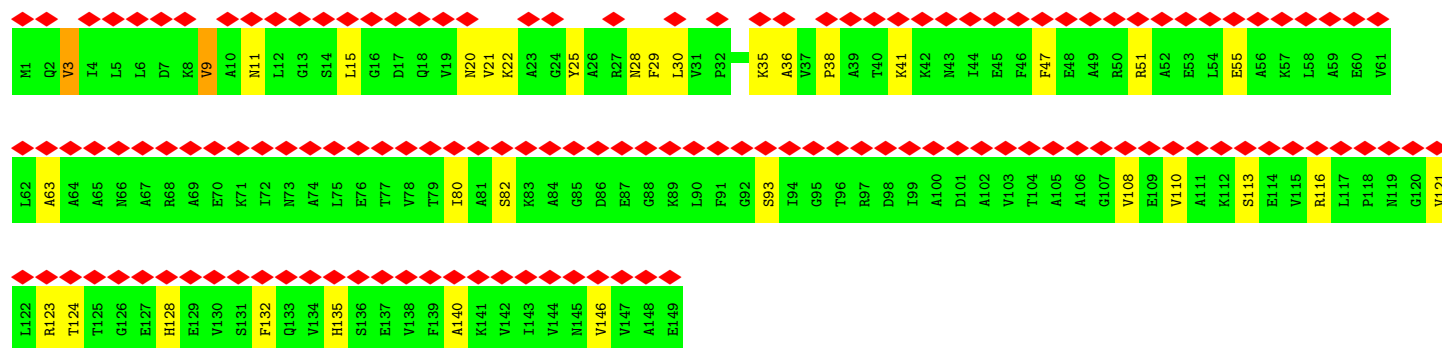
- Molecule 8: 50S ribosomal protein L7/L12

Chain 1L: 56% 57% 43%



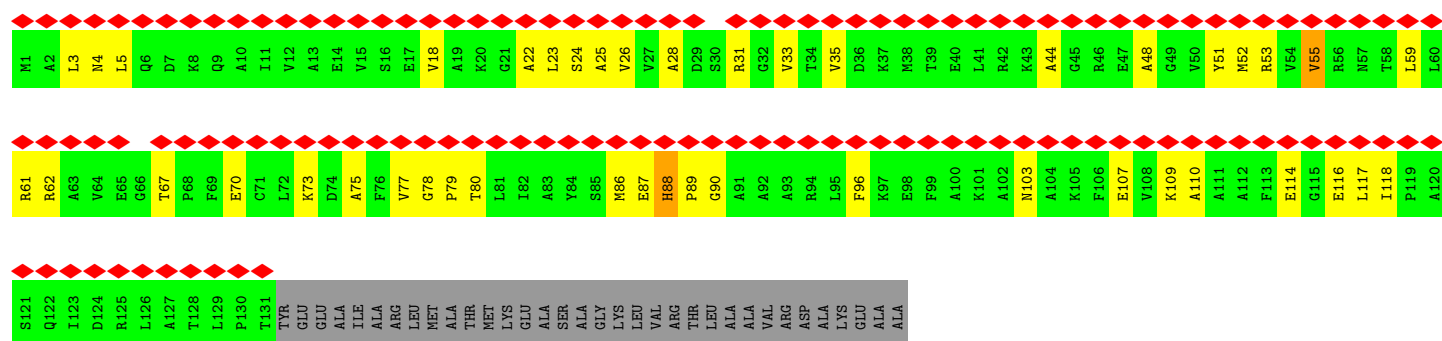
- Molecule 9: 50S ribosomal protein L9

Chain 1I: 



• Molecule 10: 50S ribosomal protein L10

Chain 1J: 



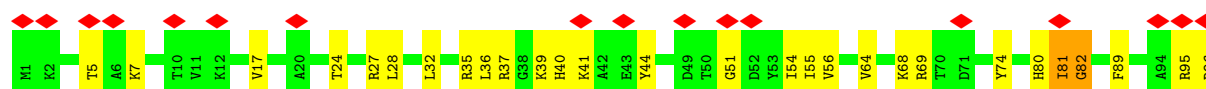
• Molecule 11: 50S ribosomal protein L11

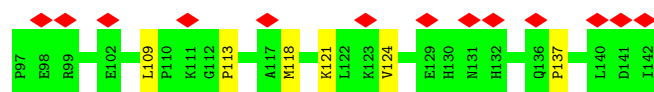
Chain 1K: 



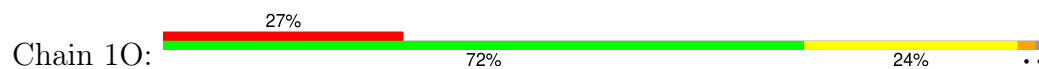
• Molecule 12: 50S ribosomal protein L13

Chain 1N: 

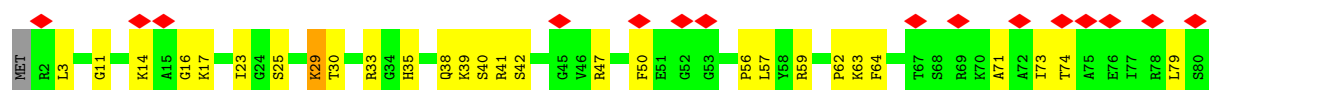
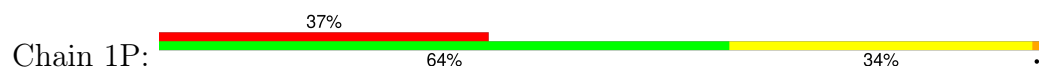




- Molecule 13: 50S ribosomal protein L14



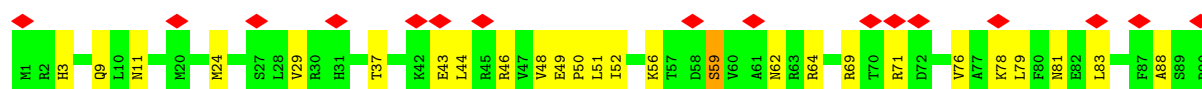
- Molecule 14: 50S ribosomal protein L15



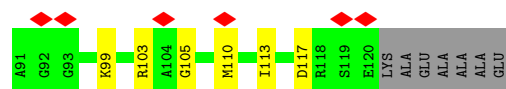
- Molecule 15: 50S ribosomal protein L16

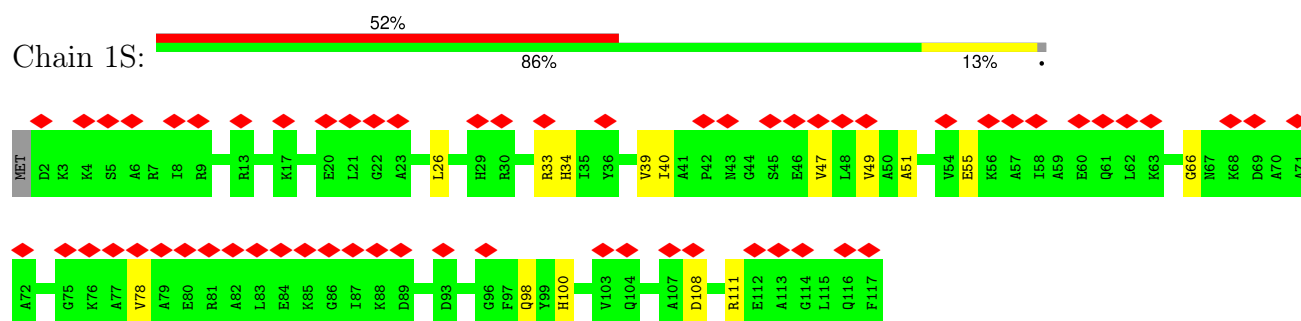


- Molecule 16: 50S ribosomal protein L17

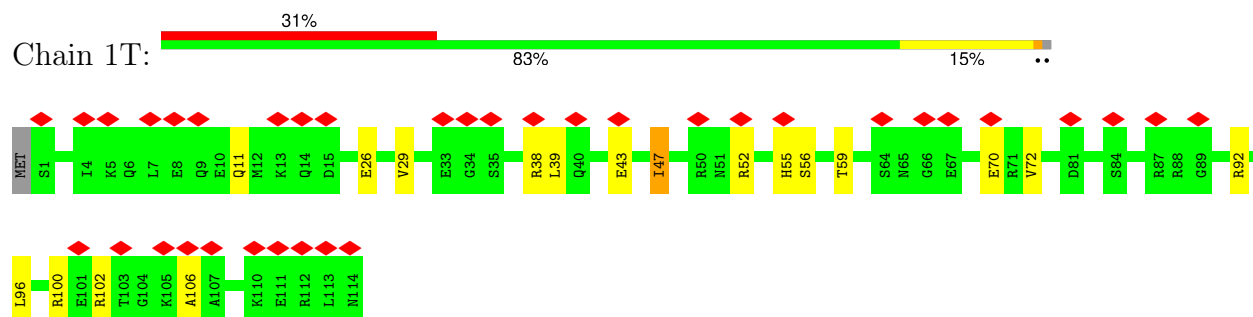


- Molecule 17: 50S ribosomal protein L18

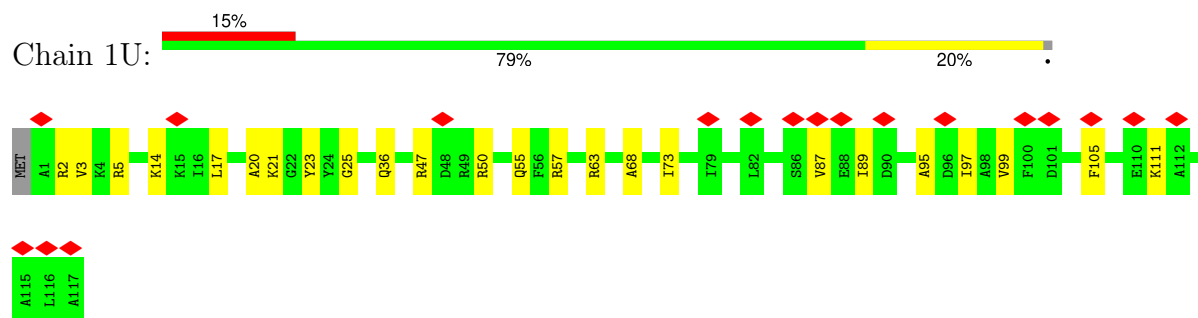




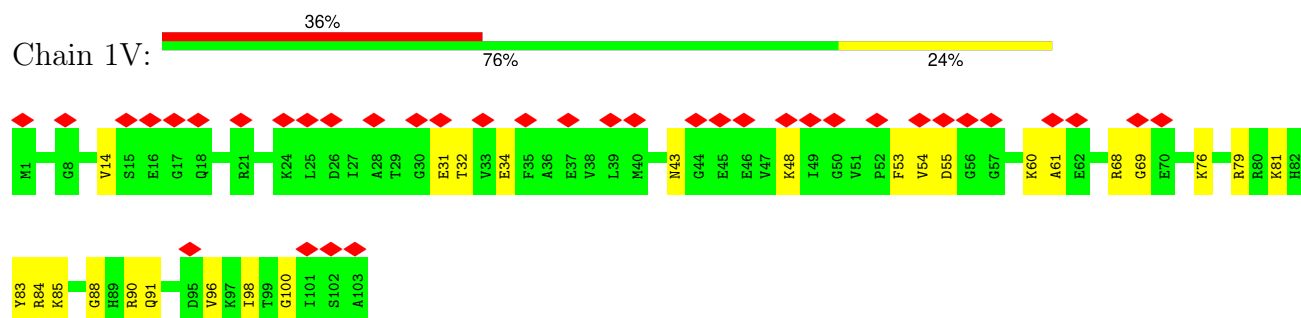
• Molecule 18: 50S ribosomal protein L19



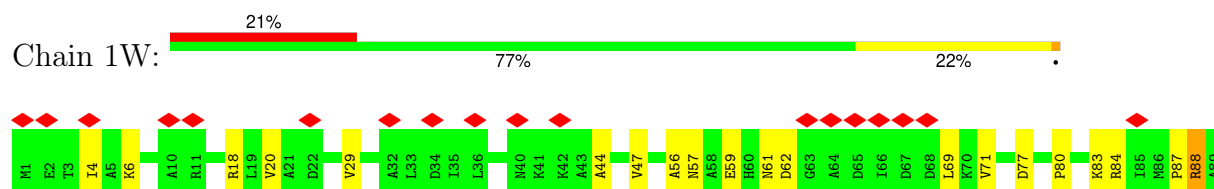
• Molecule 19: 50S ribosomal protein L20



• Molecule 20: 50S ribosomal protein L21

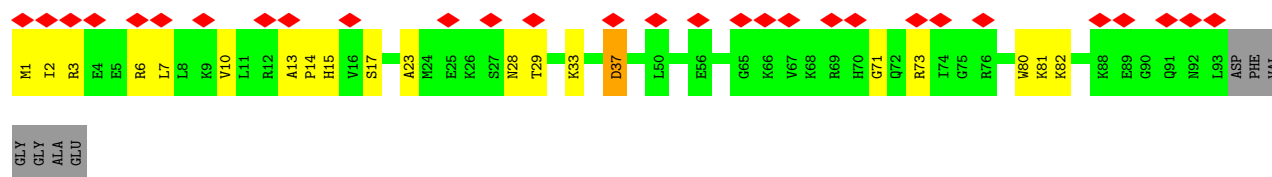
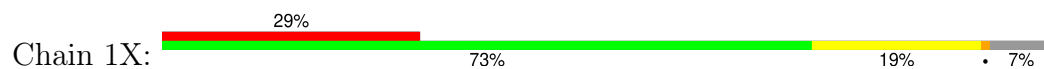


• Molecule 21: 50S ribosomal protein L22

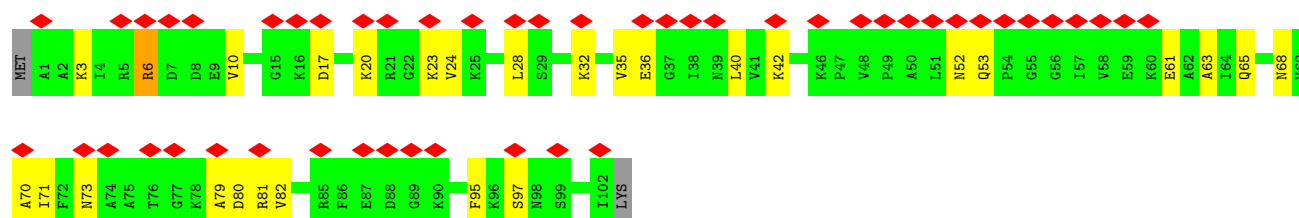
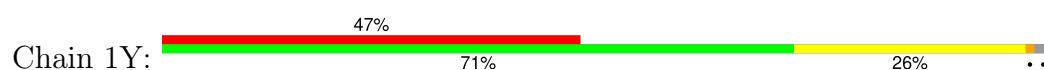




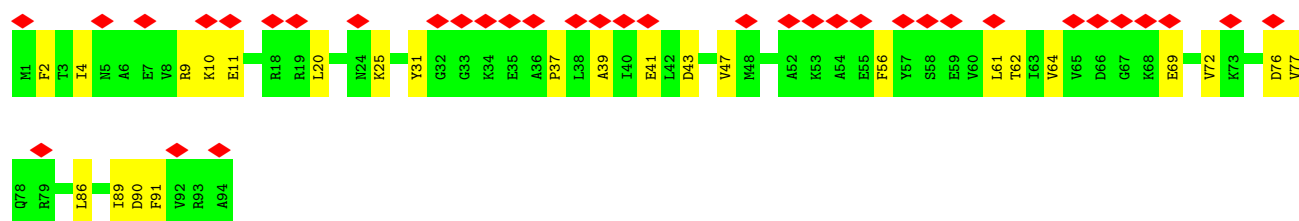
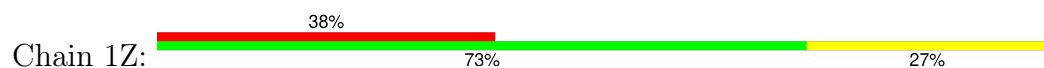
- Molecule 22: 50S ribosomal protein L23



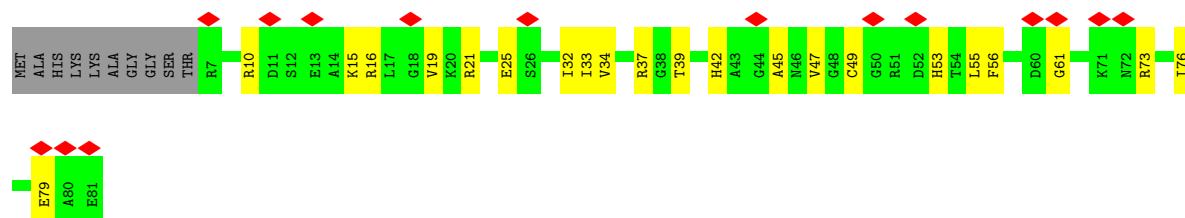
- Molecule 23: 50S ribosomal protein L24



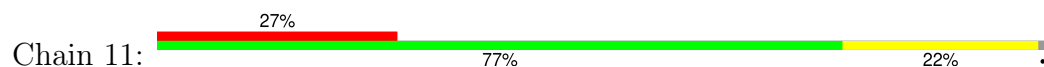
- Molecule 24: 50S ribosomal protein L25

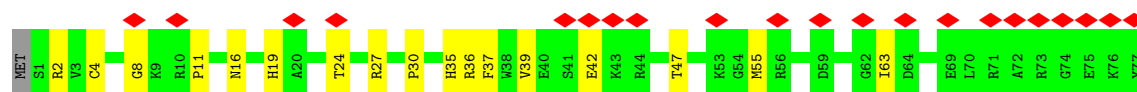


- Molecule 25: 50S ribosomal protein L27

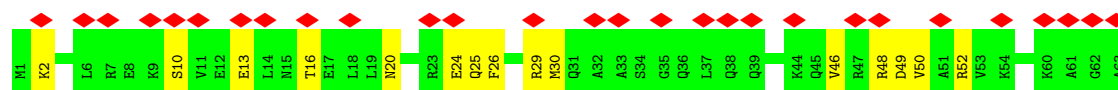
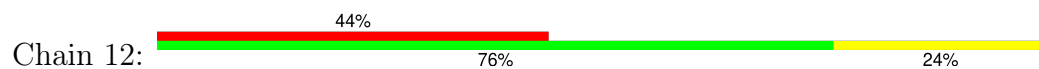


- Molecule 26: 50S ribosomal protein L28





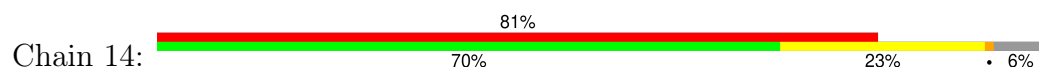
- Molecule 27: 50S ribosomal protein L29



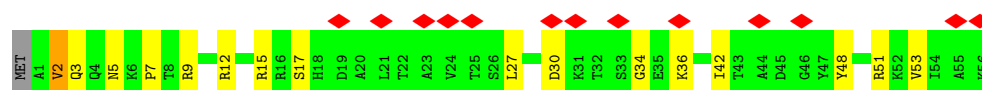
- Molecule 28: 50S ribosomal protein L30



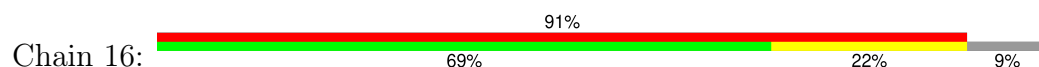
- Molecule 29: 50S ribosomal protein L31



- Molecule 30: 50S ribosomal protein L32



- Molecule 31: 50S ribosomal protein L33

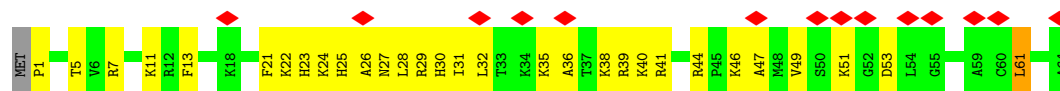


- Molecule 32: 50S ribosomal protein L34

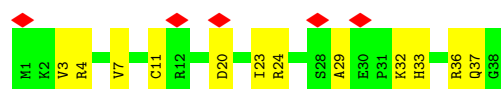




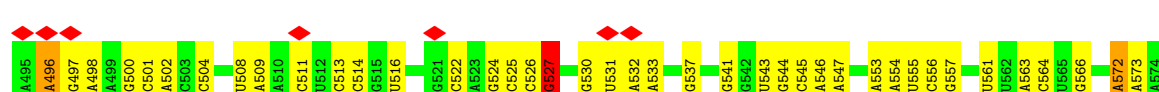
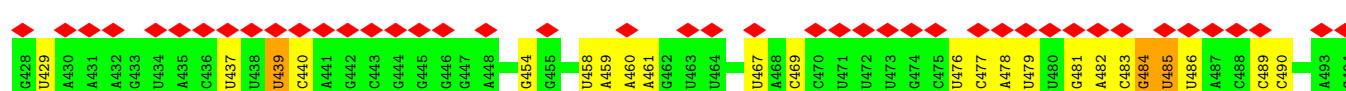
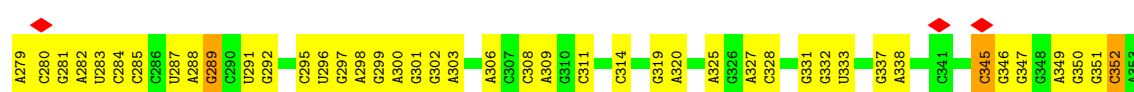
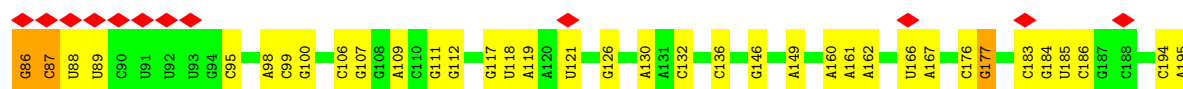
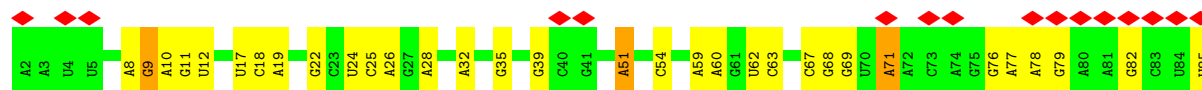
- Molecule 33: 50S ribosomal protein L35

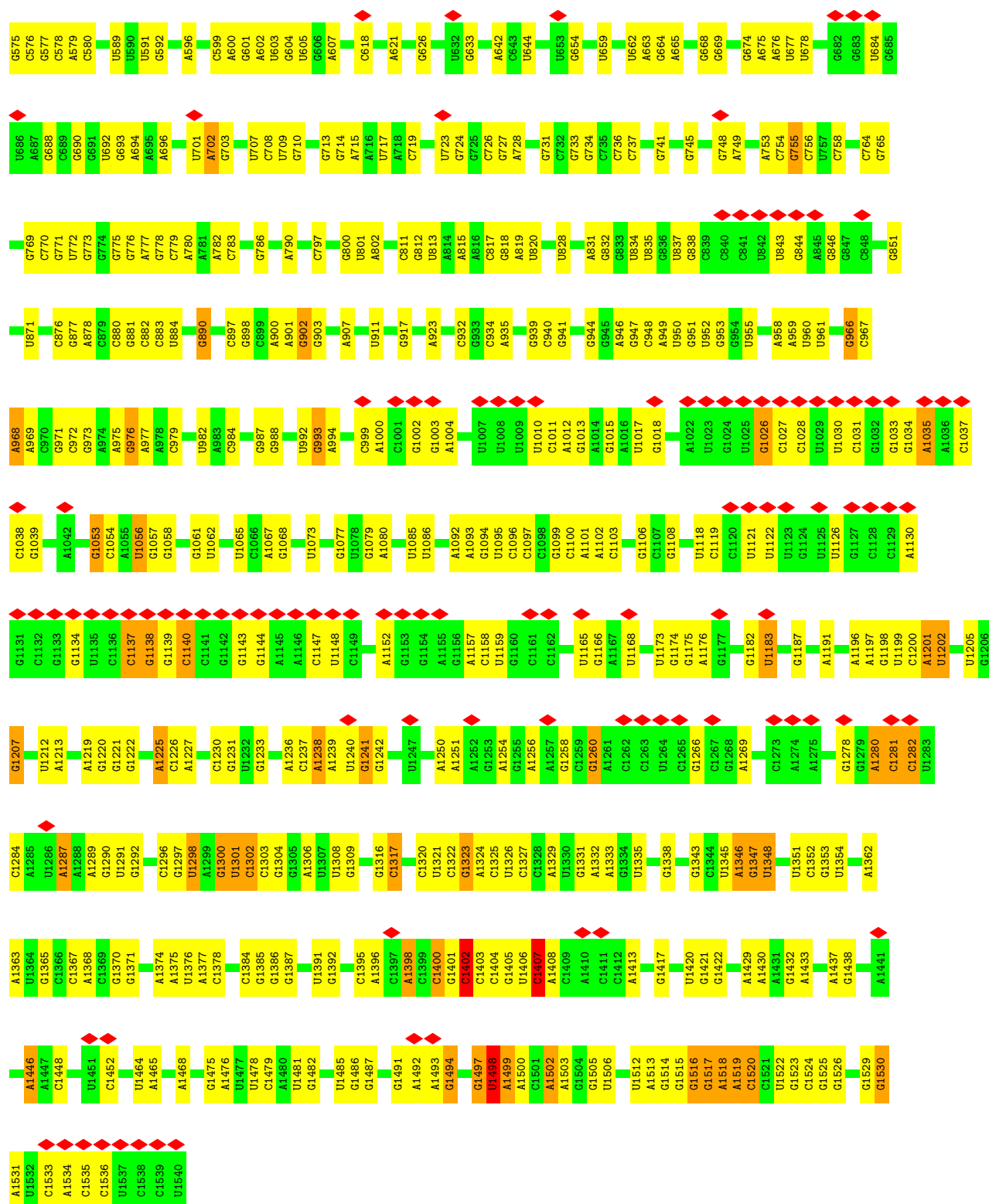


- Molecule 34: 50S ribosomal protein L36

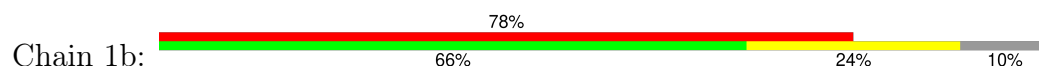


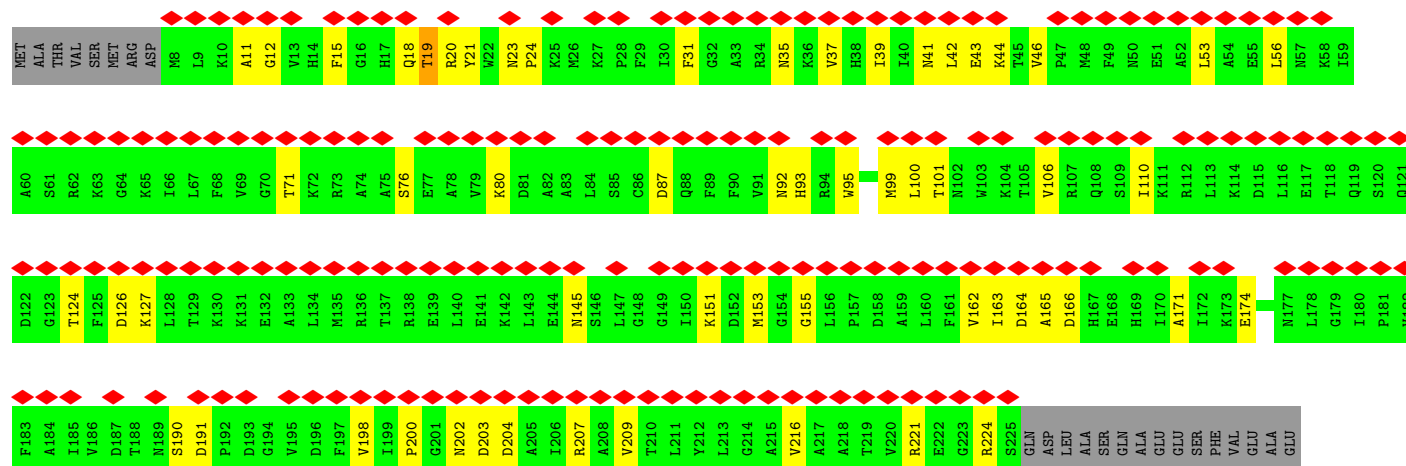
- Molecule 35: 16S Ribosomal RNA





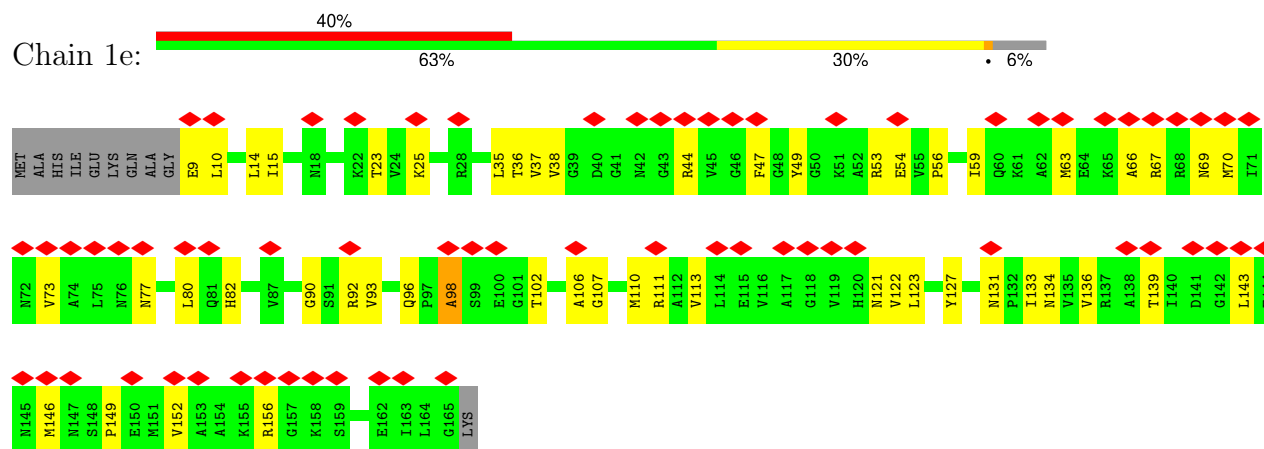
- Molecule 36: 30S ribosomal protein S2





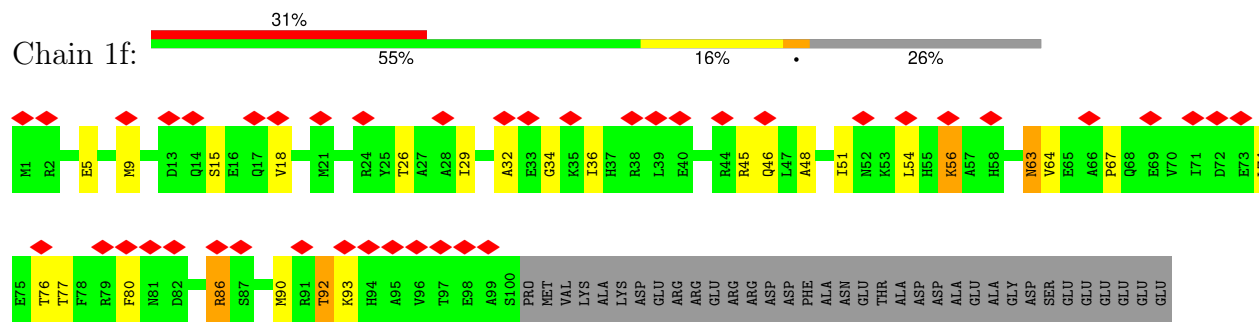
- Molecule 39: 30S ribosomal protein S5

Chain 1e:



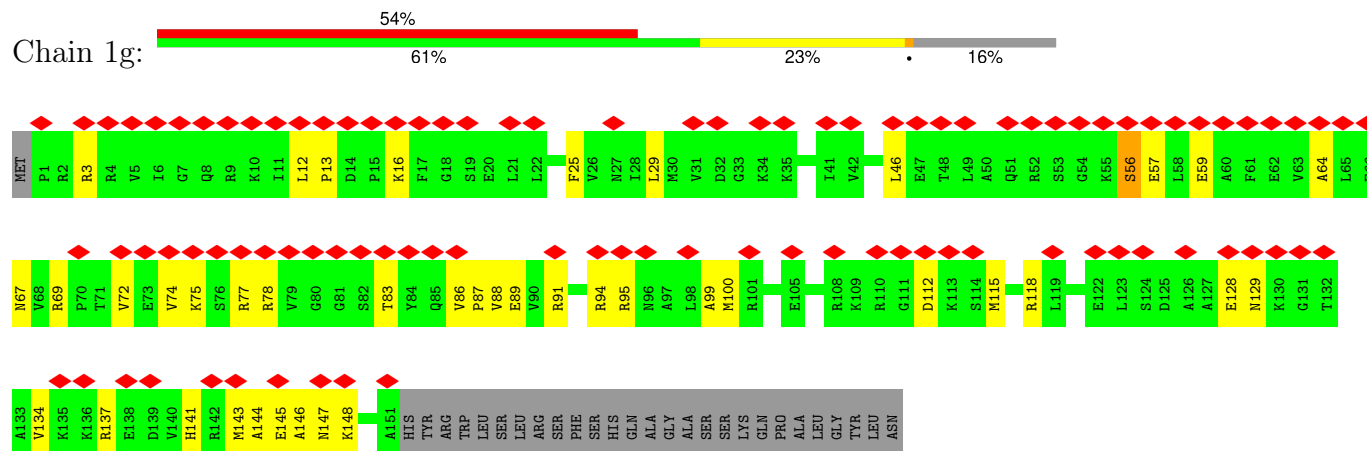
- Molecule 40: 30S ribosomal protein S6

Chain 1f:



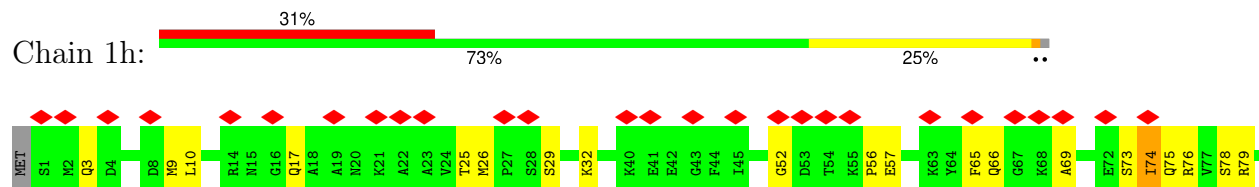
- Molecule 41: 30S ribosomal protein S7

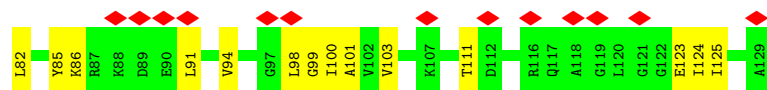
Chain 1g:



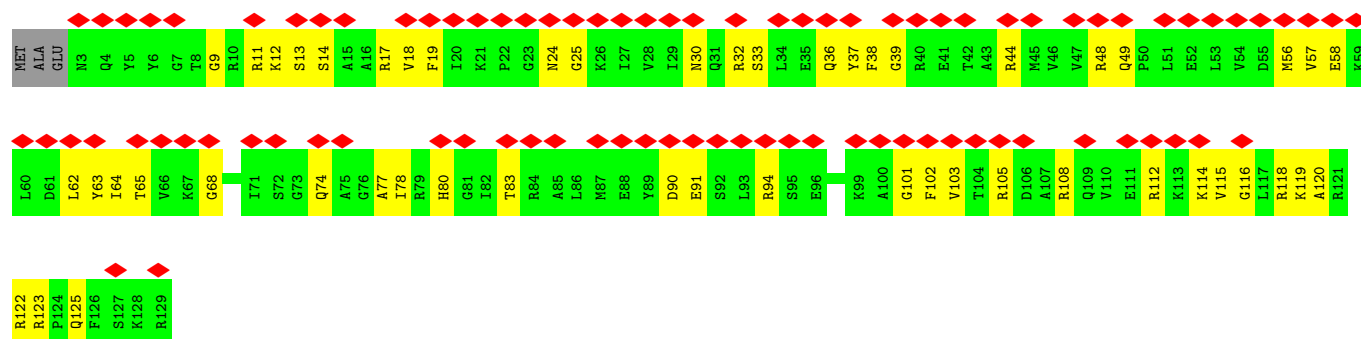
- Molecule 42: 30S ribosomal protein S8

Chain 1h:

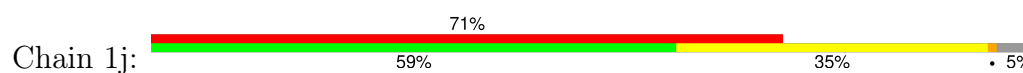




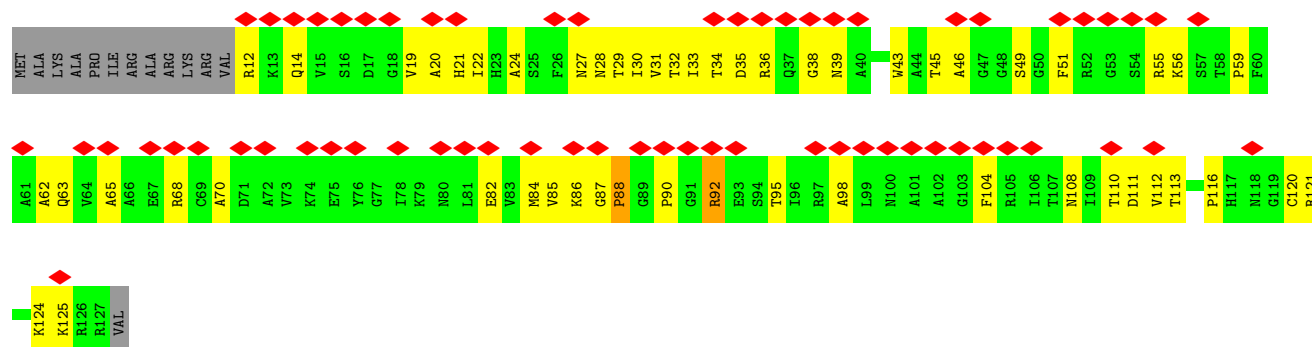
• Molecule 43: 30S ribosomal protein S9



• Molecule 44: 30S ribosomal protein S10

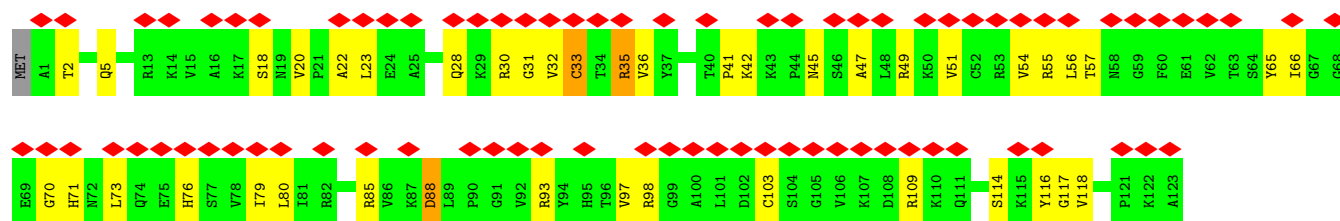


• Molecule 45: 30S ribosomal protein S11

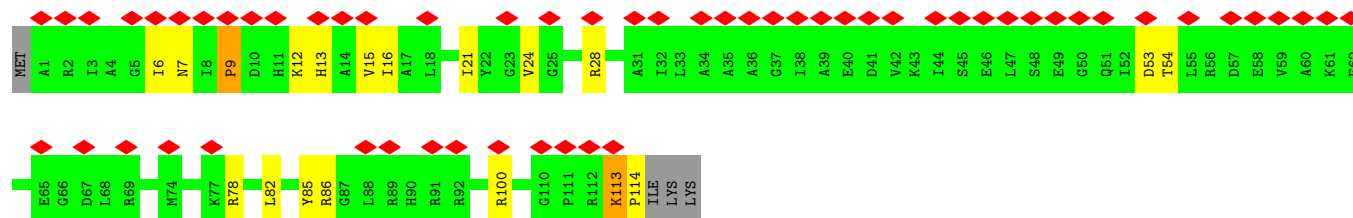
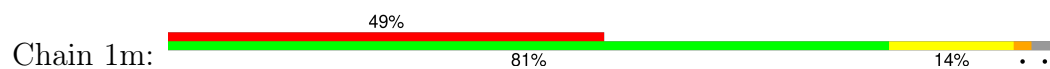


• Molecule 46: 30S ribosomal protein S12

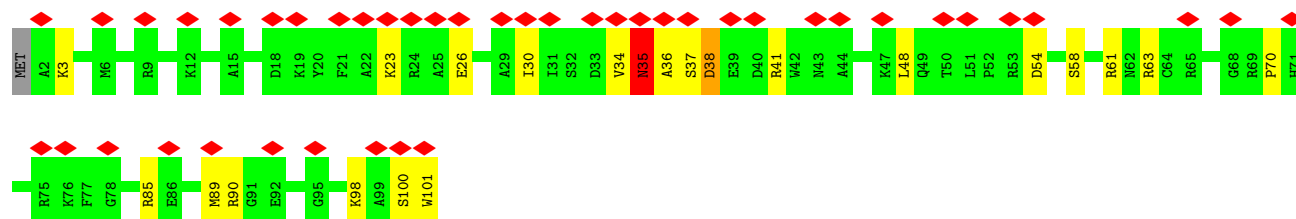
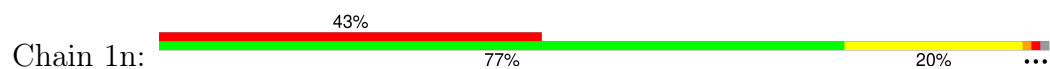




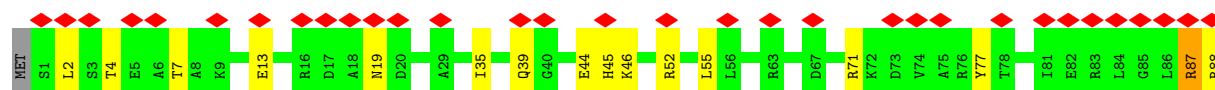
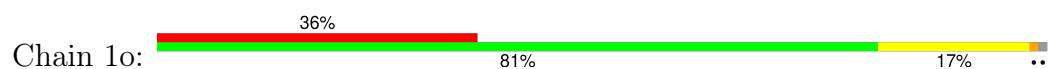
- Molecule 47: 30S ribosomal protein S13



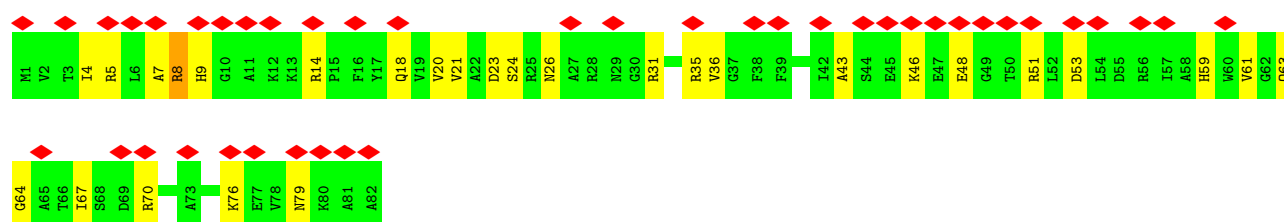
- Molecule 48: 30S ribosomal protein S14



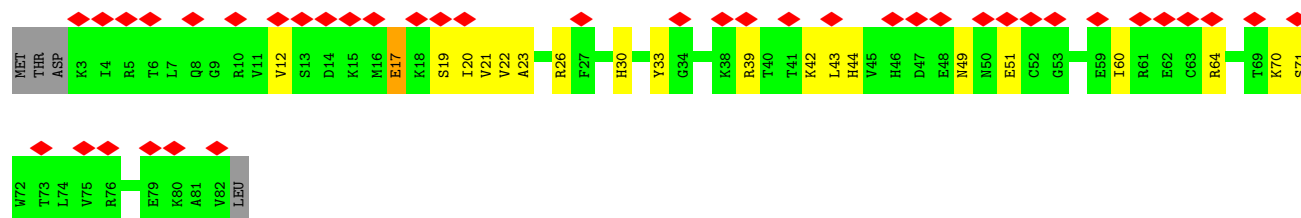
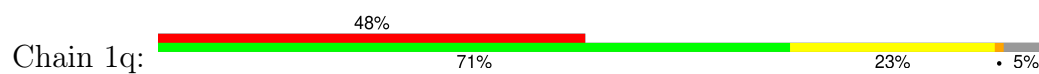
- Molecule 49: 30S ribosomal protein S15



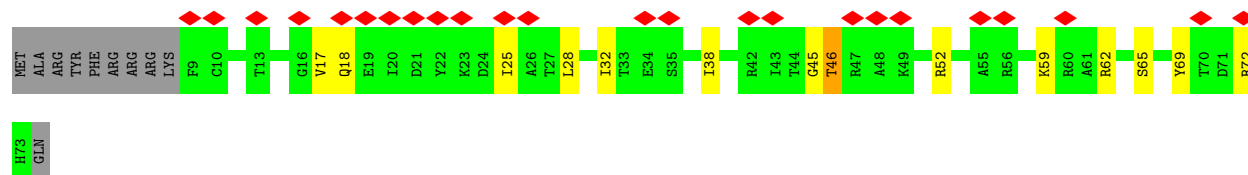
- Molecule 50: 30S ribosomal protein S16



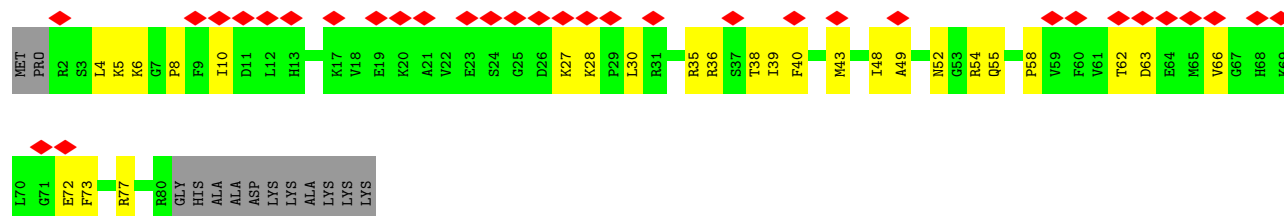
- Molecule 51: 30S ribosomal protein S17



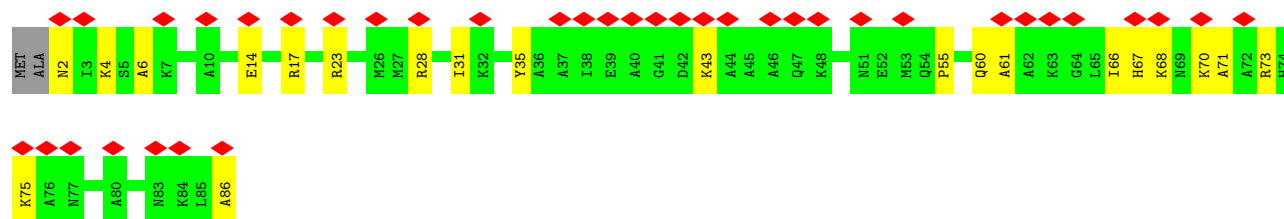
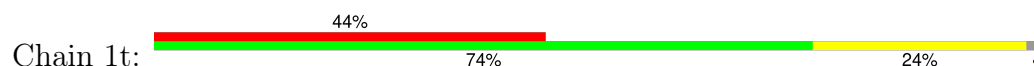
- Molecule 52: 30S ribosomal protein S18



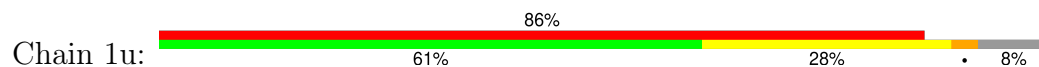
- Molecule 53: 30S ribosomal protein S19



- Molecule 54: 30S ribosomal protein S20



- Molecule 55: 30S ribosomal protein S21





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 78186                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 28                                      | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 2400                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON II (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.018                                   | Depositor |
| Minimum map value                    | -0.012                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.001                                   | Depositor |
| Recommended contour level            | 0.00307                                 | Depositor |
| Map size (Å)                         | 407.74402, 407.74402, 407.74402         | wwPDB     |
| Map dimensions                       | 368, 368, 368                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.108, 1.108, 1.108                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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   | 1A    | 0.10         | 0/69174 | 0.20        | 0/107910 |
| 2   | 1B    | 0.09         | 0/2873  | 0.19        | 0/4478   |
| 3   | 1D    | 0.21         | 0/2121  | 0.38        | 0/2852   |
| 4   | 1E    | 0.15         | 0/1586  | 0.32        | 0/2134   |
| 5   | 1F    | 0.14         | 0/1571  | 0.30        | 0/2113   |
| 6   | 1G    | 0.15         | 0/1434  | 0.34        | 0/1926   |
| 7   | 1H    | 0.15         | 0/1343  | 0.31        | 0/1816   |
| 8   | 1L    | 0.15         | 0/275   | 0.27        | 0/342    |
| 9   | 1I    | 0.16         | 0/1122  | 0.31        | 0/1515   |
| 10  | 1J    | 0.24         | 0/1001  | 0.45        | 0/1350   |
| 11  | 1K    | 0.17         | 0/1046  | 0.32        | 0/1410   |
| 12  | 1N    | 0.15         | 0/1152  | 0.33        | 0/1551   |
| 13  | 1O    | 0.16         | 0/947   | 0.38        | 0/1268   |
| 14  | 1P    | 0.16         | 0/1054  | 0.37        | 0/1403   |
| 15  | 1Q    | 0.21         | 0/1093  | 0.45        | 0/1460   |
| 16  | 1R    | 0.16         | 0/973   | 0.36        | 0/1301   |
| 17  | 1S    | 0.15         | 0/902   | 0.31        | 0/1209   |
| 18  | 1T    | 0.17         | 0/929   | 0.37        | 0/1242   |
| 19  | 1U    | 0.13         | 0/960   | 0.31        | 0/1278   |
| 20  | 1V    | 0.17         | 0/829   | 0.32        | 0/1107   |
| 21  | 1W    | 0.16         | 0/864   | 0.34        | 0/1156   |
| 22  | 1X    | 0.15         | 0/744   | 0.33        | 0/994    |
| 23  | 1Y    | 0.16         | 0/787   | 0.33        | 0/1051   |
| 24  | 1Z    | 0.18         | 0/766   | 0.37        | 0/1025   |
| 25  | 10    | 0.15         | 0/582   | 0.33        | 0/769    |
| 26  | 11    | 0.15         | 0/635   | 0.34        | 0/848    |
| 27  | 12    | 0.11         | 0/510   | 0.30        | 0/677    |
| 28  | 13    | 0.15         | 0/453   | 0.33        | 0/605    |
| 29  | 14    | 0.17         | 0/531   | 0.34        | 0/709    |
| 30  | 15    | 0.14         | 0/450   | 0.34        | 0/599    |
| 31  | 16    | 0.15         | 0/416   | 0.32        | 0/554    |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 32  | 17    | 0.14         | 0/380           | 0.37        | 0/498           |
| 33  | 18    | 0.15         | 0/513           | 0.35        | 0/676           |
| 34  | 19    | 0.14         | 0/303           | 0.35        | 0/397           |
| 35  | 1a    | 0.10         | 1/36701 (0.0%)  | 0.19        | 0/57246         |
| 36  | 1b    | 0.15         | 0/1735          | 0.33        | 0/2338          |
| 37  | 1c    | 0.18         | 0/1651          | 0.36        | 0/2225          |
| 38  | 1d    | 0.24         | 1/1665 (0.1%)   | 0.37        | 0/2227          |
| 39  | 1e    | 0.15         | 0/1154          | 0.37        | 0/1554          |
| 40  | 1f    | 0.14         | 0/835           | 0.37        | 0/1128          |
| 41  | 1g    | 0.15         | 0/1195          | 0.38        | 0/1602          |
| 42  | 1h    | 0.17         | 0/989           | 0.34        | 0/1326          |
| 43  | 1i    | 0.17         | 0/1034          | 0.41        | 0/1375          |
| 44  | 1j    | 0.18         | 0/796           | 0.41        | 0/1077          |
| 45  | 1k    | 0.16         | 0/885           | 0.36        | 0/1195          |
| 46  | 1l    | 0.18         | 0/969           | 0.40        | 0/1300          |
| 47  | 1m    | 0.16         | 0/892           | 0.37        | 0/1193          |
| 48  | 1n    | 0.16         | 0/806           | 0.39        | 0/1074          |
| 49  | 1o    | 0.14         | 0/722           | 0.31        | 0/964           |
| 50  | 1p    | 0.16         | 0/659           | 0.32        | 0/884           |
| 51  | 1q    | 0.21         | 0/657           | 0.41        | 0/881           |
| 52  | 1r    | 0.16         | 0/511           | 0.36        | 0/689           |
| 53  | 1s    | 0.13         | 0/652           | 0.31        | 0/877           |
| 54  | 1t    | 0.14         | 0/671           | 0.32        | 0/888           |
| 55  | 1u    | 0.31         | 1/500 (0.2%)    | 0.42        | 0/668           |
| 56  | 1v    | 0.23         | 0/214           | 0.36        | 0/331           |
| 57  | 1w    | 0.17         | 0/2594          | 0.39        | 6/3251 (0.2%)   |
| 58  | 1x    | 0.14         | 0/1656          | 0.20        | 0/2575          |
| All | All   | 0.13         | 3/160462 (0.0%) | 0.25        | 6/239091 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 38  | 1d    | 16   | THR  | CA-C  | 7.44 | 1.55        | 1.52     |
| 35  | 1a    | 1498 | UR3  | O3'-P | 5.36 | 1.61        | 1.56     |
| 55  | 1u    | 9    | GLU  | C-N   | 5.04 | 1.45        | 1.33     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 57  | 1w    | 439 | ASN  | CA-C-N | 6.45 | 126.40      | 119.76   |
| 57  | 1w    | 439 | ASN  | C-N-CA | 6.45 | 126.40      | 119.76   |
| 57  | 1w    | 623 | ARG  | CA-C-N | 5.24 | 126.39      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 57  | 1w    | 623 | ARG  | C-N-CA | 5.24 | 126.39      | 119.84   |
| 57  | 1w    | 436 | VAL  | CA-C-N | 5.01 | 125.54      | 120.38   |
| 57  | 1w    | 436 | VAL  | C-N-CA | 5.01 | 125.54      | 120.38   |

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   | 1A    | 62276 | 0        | 31344    | 881     | 0            |
| 2   | 1B    | 2570  | 0        | 1301     | 25      | 0            |
| 3   | 1D    | 2082  | 0        | 2157     | 77      | 0            |
| 4   | 1E    | 1565  | 0        | 1616     | 47      | 0            |
| 5   | 1F    | 1552  | 0        | 1619     | 38      | 0            |
| 6   | 1G    | 1410  | 0        | 1447     | 39      | 0            |
| 7   | 1H    | 1323  | 0        | 1374     | 17      | 0            |
| 8   | 1L    | 276   | 0        | 79       | 0       | 0            |
| 9   | 1I    | 1111  | 0        | 1148     | 20      | 0            |
| 10  | 1J    | 988   | 0        | 1025     | 25      | 0            |
| 11  | 1K    | 1032  | 0        | 1088     | 18      | 0            |
| 12  | 1N    | 1129  | 0        | 1162     | 26      | 0            |
| 13  | 1O    | 938   | 0        | 1012     | 22      | 0            |
| 14  | 1P    | 1045  | 0        | 1117     | 40      | 0            |
| 15  | 1Q    | 1074  | 0        | 1157     | 38      | 0            |
| 16  | 1R    | 960   | 0        | 1000     | 24      | 0            |
| 17  | 1S    | 892   | 0        | 923      | 9       | 0            |
| 18  | 1T    | 917   | 0        | 965      | 15      | 0            |
| 19  | 1U    | 947   | 0        | 1022     | 19      | 0            |
| 20  | 1V    | 816   | 0        | 839      | 17      | 0            |
| 21  | 1W    | 857   | 0        | 922      | 21      | 0            |
| 22  | 1X    | 738   | 0        | 807      | 12      | 0            |
| 23  | 1Y    | 779   | 0        | 834      | 19      | 0            |
| 24  | 1Z    | 753   | 0        | 780      | 16      | 0            |
| 25  | 10    | 575   | 0        | 592      | 19      | 0            |
| 26  | 11    | 625   | 0        | 655      | 15      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 27  | 12    | 509    | 0        | 543      | 10      | 0            |
| 28  | 13    | 449    | 0        | 491      | 9       | 0            |
| 29  | 14    | 522    | 0        | 522      | 15      | 0            |
| 30  | 15    | 444    | 0        | 461      | 12      | 0            |
| 31  | 16    | 409    | 0        | 440      | 9       | 0            |
| 32  | 17    | 377    | 0        | 418      | 22      | 0            |
| 33  | 18    | 504    | 0        | 574      | 25      | 0            |
| 34  | 19    | 302    | 0        | 343      | 9       | 0            |
| 35  | 1a    | 33029  | 0        | 16644    | 463     | 0            |
| 36  | 1b    | 1704   | 0        | 1732     | 34      | 0            |
| 37  | 1c    | 1624   | 0        | 1699     | 40      | 0            |
| 38  | 1d    | 1643   | 0        | 1710     | 47      | 0            |
| 39  | 1e    | 1141   | 0        | 1170     | 30      | 0            |
| 40  | 1f    | 817    | 0        | 808      | 17      | 0            |
| 41  | 1g    | 1181   | 0        | 1240     | 27      | 0            |
| 42  | 1h    | 979    | 0        | 1034     | 21      | 0            |
| 43  | 1i    | 1022   | 0        | 1070     | 37      | 0            |
| 44  | 1j    | 786    | 0        | 828      | 23      | 0            |
| 45  | 1k    | 869    | 0        | 878      | 44      | 0            |
| 46  | 1l    | 955    | 0        | 1019     | 33      | 0            |
| 47  | 1m    | 883    | 0        | 944      | 14      | 0            |
| 48  | 1n    | 794    | 0        | 833      | 12      | 0            |
| 49  | 1o    | 714    | 0        | 737      | 10      | 0            |
| 50  | 1p    | 649    | 0        | 666      | 25      | 0            |
| 51  | 1q    | 648    | 0        | 691      | 13      | 0            |
| 52  | 1r    | 504    | 0        | 502      | 10      | 0            |
| 53  | 1s    | 637    | 0        | 665      | 19      | 0            |
| 54  | 1t    | 665    | 0        | 714      | 17      | 0            |
| 55  | 1u    | 495    | 0        | 486      | 10      | 0            |
| 56  | 1v    | 192    | 0        | 98       | 6       | 0            |
| 57  | 1w    | 2590   | 0        | 731      | 4       | 0            |
| 58  | 1x    | 1567   | 0        | 798      | 24      | 0            |
| 59  | 1A    | 111    | 0        | 0        | 0       | 0            |
| All | All   | 148945 | 0        | 99474    | 2238    | 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 (2238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:827:U:H2'    | 1:1A:2068:U:O2     | 1.20                     | 1.28              |
| 1:1A:827:U:C2'    | 1:1A:2068:U:O2     | 1.98                     | 1.12              |
| 1:1A:827:U:H2'    | 1:1A:2068:U:C2     | 1.97                     | 1.00              |
| 1:1A:776:G:H22    | 1:1A:2072:C:H5'    | 1.35                     | 0.89              |
| 6:1G:140:ILE:HG22 | 6:1G:142:TYR:H     | 1.43                     | 0.84              |
| 58:1x:49:G:H1     | 58:1x:65:PSU:HN3   | 1.25                     | 0.83              |
| 2:1B:30:C:H1'     | 2:1B:57:A:H61      | 1.41                     | 0.83              |
| 14:1P:62:PRO:HB2  | 33:18:29:ARG:HH11  | 1.44                     | 0.83              |
| 35:1a:297:G:N2    | 35:1a:300:A:OP2    | 2.11                     | 0.82              |
| 56:1v:25:A:N1     | 57:1w:442:TRP:HZ2  | 1.79                     | 0.81              |
| 35:1a:898:G:N2    | 35:1a:901:A:OP2    | 2.14                     | 0.80              |
| 1:1A:1613:G:H4'   | 32:17:3:ARG:HE     | 1.46                     | 0.80              |
| 13:1O:19:VAL:HG12 | 13:1O:43:ILE:HA    | 1.62                     | 0.80              |
| 37:1c:63:ILE:HG21 | 37:1c:94:ALA:HB1   | 1.63                     | 0.80              |
| 36:1b:153:MET:HG2 | 36:1b:155:GLY:H    | 1.47                     | 0.79              |
| 5:1F:146:VAL:HG12 | 5:1F:185:LYS:HB2   | 1.64                     | 0.79              |
| 35:1a:1086:U:H3   | 35:1a:1099:G:H22   | 1.27                     | 0.79              |
| 1:1A:38:A:H4'     | 5:1F:45:ALA:HB3    | 1.63                     | 0.79              |
| 1:1A:807:U:OP2    | 14:1P:41:ARG:NH1   | 2.15                     | 0.79              |
| 1:1A:1798:U:H5''  | 3:1D:257:ARG:HB2   | 1.64                     | 0.78              |
| 1:1A:2598:A:H5''  | 3:1D:233:GLY:HA3   | 1.65                     | 0.78              |
| 1:1A:1032:A:H1'   | 34:19:23:ILE:HD13  | 1.66                     | 0.78              |
| 1:1A:198:C:H1'    | 1:1A:2434:A:H61    | 1.49                     | 0.77              |
| 39:1e:156:ARG:NH2 | 42:1h:98:LEU:O     | 2.18                     | 0.77              |
| 1:1A:827:U:C2'    | 1:1A:2068:U:C2     | 2.63                     | 0.77              |
| 35:1a:676:A:N6    | 35:1a:713:G:O6     | 2.18                     | 0.77              |
| 12:1N:80:HIS:O    | 12:1N:82:GLY:N     | 2.17                     | 0.76              |
| 58:1x:6:U:H3      | 58:1x:67:A:H61     | 1.32                     | 0.76              |
| 35:1a:1221:G:OP1  | 53:1s:35:ARG:NH1   | 2.19                     | 0.76              |
| 1:1A:574:A:N6     | 1:1A:2034:U:OP1    | 2.19                     | 0.76              |
| 35:1a:522:C:H41   | 46:1l:49:ARG:HH22  | 1.33                     | 0.76              |
| 35:1a:1516:2MG:N1 | 35:1a:1520:C:N3    | 2.35                     | 0.75              |
| 1:1A:2420:C:H2'   | 1:1A:2421:G:H8     | 1.51                     | 0.75              |
| 35:1a:955:U:H3    | 35:1a:1225:A:H61   | 1.35                     | 0.75              |
| 45:1k:87:GLY:H    | 45:1k:113:THR:HG22 | 1.51                     | 0.75              |
| 1:1A:2394:C:H5''  | 14:1P:63:LYS:HE3   | 1.68                     | 0.75              |
| 36:1b:99:MET:HA   | 36:1b:106:VAL:HG21 | 1.68                     | 0.75              |
| 1:1A:466:A:OP1    | 32:17:34:ARG:NH1   | 2.20                     | 0.74              |
| 18:1T:59:THR:HG22 | 18:1T:72:VAL:HG12  | 1.69                     | 0.74              |
| 45:1k:63:GLN:HG3  | 45:1k:98:ALA:HB2   | 1.68                     | 0.74              |
| 1:1A:275:C:O2     | 1:1A:362:A:N6      | 2.20                     | 0.74              |
| 35:1a:1266:G:N2   | 35:1a:1269:A:OP2   | 2.19                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:1a:553:A:H5''   | 46:1l:20:VAL:HG21  | 1.67                     | 0.74              |
| 1:1A:1568:G:OP2    | 3:1D:62:ARG:NH2    | 2.15                     | 0.74              |
| 35:1a:185:U:O2     | 54:1t:75:LYS:NZ    | 2.20                     | 0.74              |
| 1:1A:2484:G:OP1    | 15:1Q:44:ARG:NH2   | 2.21                     | 0.73              |
| 45:1k:86:LYS:NZ    | 45:1k:112:VAL:O    | 2.21                     | 0.73              |
| 1:1A:1992:G:N2     | 1:1A:1996:C:O2'    | 2.22                     | 0.73              |
| 24:1Z:9:ARG:HD3    | 24:1Z:39:ALA:HB1   | 1.70                     | 0.73              |
| 1:1A:320:A:N3      | 5:1F:163:ASN:ND2   | 2.36                     | 0.73              |
| 1:1A:1054:A:H61    | 1:1A:1105:U:H3     | 1.37                     | 0.73              |
| 35:1a:82:G:N2      | 35:1a:87:C:N3      | 2.37                     | 0.73              |
| 9:1I:80:ILE:HD12   | 9:1I:146:VAL:HG22  | 1.71                     | 0.72              |
| 4:1E:15:PHE:H      | 18:1T:11:GLN:HE22  | 1.37                     | 0.72              |
| 35:1a:149:A:H4'    | 35:1a:1446:A:H1'   | 1.70                     | 0.72              |
| 1:1A:1796:U:H2'    | 1:1A:1797:G:H8     | 1.55                     | 0.72              |
| 37:1c:110:LEU:HD13 | 37:1c:203:LYS:HE3  | 1.70                     | 0.72              |
| 1:1A:621:A:OP2     | 14:1P:99:ASN:ND2   | 2.23                     | 0.72              |
| 1:1A:2478:A:H5'    | 34:19:32:LYS:HE3   | 1.72                     | 0.72              |
| 1:1A:668:A:H2'     | 1:1A:670:A:H62     | 1.55                     | 0.71              |
| 1:1A:1759:A:HO2'   | 1:1A:2714:G:HO2'   | 1.29                     | 0.71              |
| 1:1A:690:G:H1      | 1:1A:772:C:H42     | 1.39                     | 0.71              |
| 1:1A:1364:G:N2     | 1:1A:1367:A:OP2    | 2.22                     | 0.71              |
| 35:1a:707:U:O2'    | 45:1k:38:GLY:O     | 2.08                     | 0.71              |
| 35:1a:1384:C:H2'   | 35:1a:1385:G:H8    | 1.56                     | 0.71              |
| 41:1g:115:MET:HA   | 41:1g:118:ARG:HE   | 1.55                     | 0.71              |
| 1:1A:2581:G:N2     | 1:1A:2581:G:OP2    | 2.24                     | 0.71              |
| 1:1A:2063:C:N4     | 1:1A:2501:C:O2     | 2.24                     | 0.71              |
| 53:1s:5:LYS:HG3    | 53:1s:6:LYS:HG2    | 1.72                     | 0.71              |
| 25:10:33:ILE:HG22  | 25:10:34:VAL:HG23  | 1.72                     | 0.71              |
| 1:1A:1864:U:OP1    | 1:1A:2410:G:O2'    | 2.09                     | 0.70              |
| 10:1J:73:LYS:HB3   | 10:1J:117:LEU:HD11 | 1.72                     | 0.70              |
| 16:1R:37:THR:HG22  | 16:1R:110:MET:HE1  | 1.72                     | 0.70              |
| 1:1A:698:C:O2'     | 1:1A:734:A:N6      | 2.23                     | 0.70              |
| 1:1A:1072:C:N3     | 1:1A:1092:C:N4     | 2.39                     | 0.70              |
| 1:1A:2251:OMG:OP1  | 15:1Q:81:ARG:NH1   | 2.23                     | 0.70              |
| 14:1P:23:ILE:HD13  | 20:1V:84:ARG:HH22  | 1.55                     | 0.70              |
| 38:1d:60:VAL:HG21  | 38:1d:199:ILE:HD11 | 1.73                     | 0.70              |
| 1:1A:291:G:H1      | 1:1A:349:U:H3      | 1.39                     | 0.70              |
| 5:1F:75:SER:HB3    | 5:1F:78:TRP:HD1    | 1.57                     | 0.70              |
| 46:1l:98:ARG:HB2   | 46:1l:116:TYR:HA   | 1.74                     | 0.70              |
| 13:1O:29:HIS:CE1   | 13:1O:31:ARG:HH12  | 2.10                     | 0.70              |
| 44:1j:36:VAL:HG22  | 44:1j:38:GLY:H     | 1.55                     | 0.70              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1837:C:O2'   | 1:1A:1927:A:N3     | 2.25                     | 0.70              |
| 13:1O:21:CYS:HA   | 13:1O:41:ILE:HG22  | 1.73                     | 0.69              |
| 35:1a:112:G:H21   | 35:1a:354:G:H5'    | 1.58                     | 0.69              |
| 35:1a:437:U:HO2'  | 38:1d:119:HIS:HD1  | 1.35                     | 0.69              |
| 44:1j:9:ARG:NH2   | 44:1j:99:GLN:OE1   | 2.25                     | 0.69              |
| 13:1O:112:PHE:HD1 | 13:1O:115:ILE:HD12 | 1.58                     | 0.69              |
| 37:1c:18:ASN:ND2  | 48:1n:90:ARG:O     | 2.26                     | 0.69              |
| 1:1A:192:C:O2'    | 1:1A:802:A:N3      | 2.23                     | 0.69              |
| 1:1A:1799:G:N2    | 1:1A:1819:A:OP2    | 2.20                     | 0.69              |
| 41:1g:77:ARG:HB2  | 41:1g:86:VAL:HG21  | 1.73                     | 0.69              |
| 44:1j:52:LEU:HD21 | 44:1j:59:LYS:HD2   | 1.73                     | 0.69              |
| 1:1A:1416:G:O2'   | 1:1A:1587:G:N2     | 2.26                     | 0.69              |
| 32:17:15:SER:O    | 32:17:21:ARG:NH2   | 2.25                     | 0.69              |
| 39:1e:98:ALA:HB2  | 39:1e:123:LEU:HG   | 1.74                     | 0.69              |
| 1:1A:910:A:H62    | 15:1Q:12:MET:HA    | 1.58                     | 0.69              |
| 1:1A:1614:A:H61   | 21:1W:88:ARG:H     | 1.41                     | 0.69              |
| 1:1A:1992:G:O2'   | 1:1A:1997:C:N4     | 2.26                     | 0.69              |
| 36:1b:221:ARG:HG3 | 36:1b:224:ARG:HH11 | 1.58                     | 0.69              |
| 13:1O:121:GLU:HG2 | 13:1O:122:VAL:HG23 | 1.73                     | 0.68              |
| 35:1a:18:C:OP1    | 39:1e:131:ASN:ND2  | 2.26                     | 0.68              |
| 6:1G:134:GLN:NE2  | 6:1G:149:ARG:O     | 2.26                     | 0.68              |
| 22:1X:1:MET:HG3   | 22:1X:3:ARG:H      | 1.58                     | 0.68              |
| 35:1a:136:C:O2'   | 50:1p:64:GLY:O     | 2.11                     | 0.68              |
| 38:1d:94:GLU:HA   | 38:1d:99:ASN:HD22  | 1.58                     | 0.68              |
| 1:1A:1787:A:OP1   | 3:1D:237:ARG:NH2   | 2.26                     | 0.68              |
| 1:1A:1501:G:OP1   | 3:1D:100:ARG:NH2   | 2.26                     | 0.68              |
| 1:1A:2279:G:HO2'  | 1:1A:2327:A:HO2'   | 1.28                     | 0.68              |
| 35:1a:1404:C:H2'  | 35:1a:1405:G:C8    | 2.28                     | 0.68              |
| 46:1l:41:PRO:HD2  | 46:1l:47:ALA:H     | 1.56                     | 0.68              |
| 35:1a:951:G:OP2   | 47:1m:100:ARG:NH2  | 2.26                     | 0.68              |
| 45:1k:19:VAL:N    | 45:1k:34:THR:O     | 2.23                     | 0.68              |
| 1:1A:674:G:H5''   | 5:1F:71:GLY:H      | 1.58                     | 0.68              |
| 35:1a:944:G:N1    | 35:1a:1338:G:OP2   | 2.26                     | 0.68              |
| 35:1a:1269:A:HO2' | 35:1a:1325:C:HO2'  | 1.42                     | 0.68              |
| 6:1G:1:ALA:N      | 6:1G:97:GLU:OE1    | 2.28                     | 0.67              |
| 42:1h:29:SER:HB3  | 42:1h:32:LYS:HG2   | 1.75                     | 0.67              |
| 1:1A:465:G:OP1    | 32:17:12:ARG:NH1   | 2.25                     | 0.67              |
| 5:1F:45:ALA:HB2   | 5:1F:89:PRO:HD3    | 1.76                     | 0.67              |
| 35:1a:1222:G:OP2  | 35:1a:1322:C:N4    | 2.22                     | 0.67              |
| 50:1p:4:ILE:HG12  | 50:1p:21:VAL:HG22  | 1.76                     | 0.67              |
| 1:1A:518:G:OP1    | 21:1W:18:ARG:NH1   | 2.25                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:1V:34:GLU:HG2  | 20:1V:60:LYS:HG2   | 1.74                     | 0.67              |
| 36:1b:18:GLN:NE2  | 36:1b:21:TYR:OH    | 2.26                     | 0.67              |
| 1:1A:669:G:N2     | 1:1A:672:C:OP1     | 2.27                     | 0.67              |
| 1:1A:51:G:H4'     | 1:1A:52:A:H5'      | 1.76                     | 0.67              |
| 1:1A:1945:G:N2    | 1:1A:1963:U:O4     | 2.27                     | 0.67              |
| 38:1d:94:GLU:HG2  | 38:1d:185:PRO:HG2  | 1.77                     | 0.67              |
| 1:1A:190:A:H5''   | 1:1A:204:A:H61     | 1.60                     | 0.67              |
| 1:1A:1158:C:H5''  | 28:13:30:ARG:HD2   | 1.75                     | 0.67              |
| 10:1J:33:VAL:HG12 | 10:1J:35:VAL:H     | 1.59                     | 0.67              |
| 13:1O:9:ASN:OD1   | 13:1O:18:ARG:NH1   | 2.28                     | 0.67              |
| 1:1A:658:U:O2'    | 5:1F:97:ASN:OD1    | 2.12                     | 0.67              |
| 1:1A:1309:G:H4'   | 32:17:7:PRO:HG2    | 1.75                     | 0.67              |
| 29:14:26:SER:OG   | 29:14:27:THR:N     | 2.27                     | 0.67              |
| 35:1a:745:G:OP1   | 35:1a:851:G:O2'    | 2.13                     | 0.67              |
| 44:1j:40:ILE:HB   | 44:1j:73:LEU:HB2   | 1.76                     | 0.67              |
| 1:1A:1046:A:H4'   | 10:1J:61:ARG:HB3   | 1.77                     | 0.67              |
| 4:1E:110:THR:HB   | 4:1E:202:ILE:HB    | 1.76                     | 0.67              |
| 13:1O:43:ILE:HD12 | 13:1O:56:ASP:HB2   | 1.77                     | 0.67              |
| 16:1R:43:GLU:OE2  | 16:1R:46:ARG:NH2   | 2.28                     | 0.67              |
| 35:1a:1514:G:H2'  | 35:1a:1515:G:H8    | 1.60                     | 0.67              |
| 36:1b:76:SER:HB2  | 36:1b:92:ASN:HB2   | 1.75                     | 0.67              |
| 1:1A:45:G:H5''    | 1:1A:46:G:H5'      | 1.76                     | 0.66              |
| 1:1A:2118:U:O2    | 1:1A:2145:C:N4     | 2.28                     | 0.66              |
| 46:1l:35:ARG:NH1  | 46:1l:36:VAL:O     | 2.28                     | 0.66              |
| 37:1c:15:LYS:NZ   | 37:1c:182:ASP:OD1  | 2.27                     | 0.66              |
| 1:1A:1022:G:N2    | 1:1A:1023:U:O4     | 2.28                     | 0.66              |
| 35:1a:618:C:H1'   | 50:1p:14:ARG:HH12  | 1.61                     | 0.66              |
| 35:1a:1384:C:H2'  | 35:1a:1385:G:C8    | 2.30                     | 0.66              |
| 45:1k:84:MET:SD   | 45:1k:110:THR:OG1  | 2.54                     | 0.66              |
| 13:1O:30:ARG:NH2  | 13:1O:37:ASP:OD2   | 2.25                     | 0.66              |
| 35:1a:946:A:O2'   | 35:1a:1333:A:N3    | 2.27                     | 0.66              |
| 58:1x:63:A:H2'    | 58:1x:64:C:C6      | 2.30                     | 0.66              |
| 14:1P:93:ASN:O    | 14:1P:95:LEU:N     | 2.29                     | 0.66              |
| 35:1a:1200:C:H5'' | 35:1a:1201:A:H3'   | 1.78                     | 0.66              |
| 36:1b:23:ASN:ND2  | 36:1b:191:ASP:OD1  | 2.27                     | 0.66              |
| 1:1A:2618:G:H21   | 4:1E:155:VAL:HG21  | 1.60                     | 0.66              |
| 1:1A:953:G:H2'    | 1:1A:954:G:H8      | 1.61                     | 0.66              |
| 1:1A:2591:C:H2'   | 1:1A:2592:G:H8     | 1.61                     | 0.66              |
| 35:1a:1297:G:N2   | 35:1a:1298:U:O4    | 2.28                     | 0.66              |
| 1:1A:568:U:H1'    | 1:1A:2030:6MZ:H9C1 | 1.78                     | 0.65              |
| 1:1A:993:G:OP2    | 19:1U:50:ARG:NH2   | 2.27                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1394:U:H4'   | 1:1A:1603:A:H4'    | 1.78                     | 0.65              |
| 1:1A:1784:A:O2'   | 1:1A:1981:A:N7     | 2.27                     | 0.65              |
| 35:1a:554:A:OP1   | 46:1l:18:SER:OG    | 2.09                     | 0.65              |
| 39:1e:54:GLU:HG2  | 39:1e:56:PRO:HD2   | 1.79                     | 0.65              |
| 1:1A:807:U:H1'    | 1:1A:2445:2MG:OP1  | 1.96                     | 0.65              |
| 38:1d:37:PRO:HD2  | 38:1d:41:GLY:HA3   | 1.78                     | 0.65              |
| 45:1k:21:HIS:N    | 45:1k:32:THR:O     | 2.29                     | 0.65              |
| 1:1A:1378:A:H4'   | 1:1A:1379:U:OP1    | 1.97                     | 0.65              |
| 1:1A:2523:G:HO2'  | 1:1A:2764:A:HO2'   | 1.44                     | 0.65              |
| 1:1A:1060:U:H5'   | 1:1A:1062:G:H5'    | 1.79                     | 0.65              |
| 1:1A:2656:U:H2'   | 1:1A:2657:A:H8     | 1.62                     | 0.65              |
| 1:1A:2816:G:H5''  | 16:1R:99:LYS:HE2   | 1.77                     | 0.65              |
| 35:1a:51:A:H61    | 35:1a:314:C:H1'    | 1.62                     | 0.65              |
| 35:1a:331:G:O2'   | 54:1t:2:ASN:ND2    | 2.30                     | 0.65              |
| 46:1l:33:CYS:HA   | 46:1l:54:VAL:HA    | 1.79                     | 0.65              |
| 35:1a:401:C:O2'   | 35:1a:621:A:N3     | 2.29                     | 0.65              |
| 35:1a:1346:A:H2   | 43:1i:108:ARG:HH22 | 1.45                     | 0.65              |
| 38:1d:61:ARG:O    | 38:1d:65:GLY:N     | 2.30                     | 0.65              |
| 1:1A:1670:C:O2    | 4:1E:134:HIS:NE2   | 2.30                     | 0.65              |
| 1:1A:1824:G:H5''  | 3:1D:51:ARG:HH21   | 1.61                     | 0.65              |
| 1:1A:2418:A:OP1   | 33:18:44:ARG:NH2   | 2.30                     | 0.65              |
| 24:1Z:64:VAL:HG22 | 24:1Z:69:GLU:HG2   | 1.79                     | 0.65              |
| 35:1a:59:A:H5''   | 35:1a:387:U:H5''   | 1.78                     | 0.65              |
| 38:1d:14:GLU:HG3  | 38:1d:18:LEU:HD21  | 1.78                     | 0.65              |
| 1:1A:1787:A:H5''  | 3:1D:237:ARG:HH21  | 1.62                     | 0.64              |
| 35:1a:579:A:H5'   | 35:1a:728:A:H1'    | 1.78                     | 0.64              |
| 1:1A:1365:A:O4'   | 26:1l:27:ARG:NH2   | 2.29                     | 0.64              |
| 1:1A:2688:G:N1    | 1:1A:2720:U:OP2    | 2.28                     | 0.64              |
| 21:1W:57:ASN:OD1  | 21:1W:61:ASN:ND2   | 2.30                     | 0.64              |
| 28:13:12:ALA:HB1  | 28:13:20:LYS:HG2   | 1.79                     | 0.64              |
| 51:1q:23:ALA:HA   | 51:1q:42:LYS:HA    | 1.79                     | 0.64              |
| 56:1v:25:A:N1     | 57:1w:442:TRP:CZ2  | 2.65                     | 0.64              |
| 1:1A:2305:U:H5''  | 6:1G:130:GLY:HA3   | 1.80                     | 0.64              |
| 7:1H:94:ARG:HB2   | 7:1H:105:SER:HB2   | 1.80                     | 0.64              |
| 36:1b:15:PHE:HB2  | 36:1b:39:ILE:HG23  | 1.80                     | 0.64              |
| 35:1a:69:G:O6     | 35:1a:98:A:N6      | 2.30                     | 0.64              |
| 5:1F:76:PRO:HA    | 5:1F:82:GLY:HA3    | 1.78                     | 0.64              |
| 35:1a:754:C:OP1   | 49:1o:71:ARG:NH2   | 2.29                     | 0.64              |
| 58:1x:64:C:H2'    | 58:1x:65:PSU:H6    | 1.63                     | 0.64              |
| 25:10:15:LYS:HG3  | 25:10:37:ARG:HH22  | 1.63                     | 0.64              |
| 1:1A:624:C:O2'    | 1:1A:657:U:OP1     | 2.16                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:1F:41:GLN:NE2   | 5:1F:43:THR:OG1    | 2.31                     | 0.64              |
| 32:17:39:ARG:HG2  | 32:17:41:ARG:H     | 1.62                     | 0.64              |
| 38:1d:124:VAL:HA  | 38:1d:142:VAL:HA   | 1.79                     | 0.64              |
| 15:1Q:66:ARG:NH1  | 15:1Q:104:GLU:OE2  | 2.31                     | 0.63              |
| 45:1k:22:ILE:HB   | 45:1k:85:VAL:HA    | 1.80                     | 0.63              |
| 12:1N:32:LEU:HD22 | 12:1N:54:ILE:HG21  | 1.80                     | 0.63              |
| 22:1X:23:ALA:O    | 22:1X:28:ASN:N     | 2.31                     | 0.63              |
| 54:1t:4:LYS:HG3   | 54:1t:6:ALA:H      | 1.62                     | 0.63              |
| 1:1A:743:A:O2'    | 1:1A:1659:G:OP1    | 2.16                     | 0.63              |
| 1:1A:1418:G:N1    | 1:1A:1579:A:OP2    | 2.26                     | 0.63              |
| 41:1g:74:VAL:HA   | 41:1g:87:PRO:HA    | 1.81                     | 0.63              |
| 50:1p:7:ALA:HB3   | 50:1p:18:GLN:HB2   | 1.81                     | 0.63              |
| 6:1G:57:ALA:HB1   | 29:14:7:PRO:HG3    | 1.80                     | 0.63              |
| 51:1q:30:HIS:HD2  | 51:1q:33:TYR:H     | 1.47                     | 0.63              |
| 1:1A:806:C:O2     | 1:1A:2444:G:O2'    | 2.15                     | 0.63              |
| 41:1g:144:ALA:O   | 41:1g:146:ALA:N    | 2.31                     | 0.63              |
| 37:1c:65:VAL:HB   | 37:1c:100:ILE:HG22 | 1.79                     | 0.63              |
| 16:1R:44:LEU:HD23 | 16:1R:113:ILE:HD13 | 1.80                     | 0.63              |
| 1:1A:445:C:O2'    | 1:1A:449:A:N3      | 2.29                     | 0.63              |
| 1:1A:471:A:OP1    | 5:1F:79:ARG:NH1    | 2.29                     | 0.63              |
| 29:14:11:GLU:HA   | 29:14:25:ARG:HA    | 1.81                     | 0.63              |
| 44:1j:11:LYS:HE2  | 44:1j:71:LEU:HG    | 1.80                     | 0.63              |
| 25:10:21:ARG:HB2  | 25:10:33:ILE:HG23  | 1.81                     | 0.63              |
| 1:1A:745:1MG:O2'  | 1:1A:748:G:H1'     | 1.98                     | 0.62              |
| 1:1A:750:A:OP1    | 1:1A:1615:C:N4     | 2.29                     | 0.62              |
| 1:1A:1423:G:H2'   | 1:1A:1424:G:H8     | 1.64                     | 0.62              |
| 26:11:36:ARG:HA   | 26:11:47:THR:HA    | 1.80                     | 0.62              |
| 35:1a:1187:G:H4'  | 43:1i:112:ARG:HH11 | 1.64                     | 0.62              |
| 1:1A:225:C:H2'    | 1:1A:226:A:O4'     | 1.99                     | 0.62              |
| 1:1A:824:U:O2'    | 1:1A:2358:A:N6     | 2.32                     | 0.62              |
| 3:1D:77:VAL:HG22  | 3:1D:93:VAL:HG22   | 1.81                     | 0.62              |
| 1:1A:210:C:OP1    | 32:17:29:GLN:NE2   | 2.32                     | 0.62              |
| 1:1A:1309:G:O2'   | 1:1A:1611:C:O2'    | 2.17                     | 0.62              |
| 2:1B:116:G:H5'    | 17:1S:55:GLU:HG2   | 1.82                     | 0.62              |
| 1:1A:749:A:H5'    | 1:1A:1271:G:H1'    | 1.80                     | 0.62              |
| 1:1A:1323:C:N4    | 1:1A:1324:G:O6     | 2.32                     | 0.62              |
| 17:1S:108:ASP:OD1 | 17:1S:111:ARG:NH1  | 2.32                     | 0.62              |
| 29:14:28:VAL:HG11 | 29:14:32:LEU:HD13  | 1.79                     | 0.62              |
| 31:16:26:LYS:NZ   | 31:16:30:PRO:O     | 2.32                     | 0.62              |
| 35:1a:1073:U:H3   | 35:1a:1102:A:H61   | 1.47                     | 0.62              |
| 58:1x:22:G:N7     | 58:1x:46:7MG:N2    | 2.40                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1656:C:OP1    | 4:1E:141:ARG:NE    | 2.20                     | 0.62              |
| 36:1b:31:PHE:HE2   | 36:1b:41:ASN:HB2   | 1.64                     | 0.62              |
| 45:1k:20:ALA:HA    | 45:1k:33:ILE:HA    | 1.82                     | 0.62              |
| 1:1A:1835:2MG:H2'  | 1:1A:1836:C:C6     | 2.33                     | 0.62              |
| 23:1Y:28:LEU:HD12  | 23:1Y:32:LYS:HB2   | 1.81                     | 0.62              |
| 35:1a:952:U:H2'    | 35:1a:953:G:H8     | 1.65                     | 0.62              |
| 1:1A:2059:A:C8     | 1:1A:2503:2MA:HM22 | 2.34                     | 0.62              |
| 35:1a:176:C:OP1    | 54:1t:23:ARG:NH1   | 2.32                     | 0.62              |
| 1:1A:572:A:H61     | 1:1A:2029:G:H21    | 1.48                     | 0.62              |
| 1:1A:684:G:OP1     | 32:17:21:ARG:NH1   | 2.31                     | 0.62              |
| 38:1d:117:VAL:HG22 | 38:1d:122:ILE:HG13 | 1.82                     | 0.62              |
| 1:1A:1923:U:OP1    | 58:1x:24:G:O2'     | 2.17                     | 0.62              |
| 35:1a:1514:G:H2'   | 35:1a:1515:G:C8    | 2.34                     | 0.62              |
| 1:1A:784:G:C5      | 3:1D:227:VAL:HG11  | 2.35                     | 0.62              |
| 1:1A:1199:U:H1'    | 19:1U:3:VAL:HG22   | 1.82                     | 0.62              |
| 1:1A:1813:G:O2'    | 3:1D:49:THR:OG1    | 2.10                     | 0.62              |
| 1:1A:2057:G:H1'    | 30:15:2:VAL:HG21   | 1.81                     | 0.62              |
| 1:1A:2298:A:OP1    | 6:1G:70:ARG:NH2    | 2.31                     | 0.62              |
| 2:1B:76:G:OP1      | 24:1Z:9:ARG:NH2    | 2.29                     | 0.62              |
| 6:1G:56:LEU:HB2    | 6:1G:64:PRO:HG3    | 1.81                     | 0.62              |
| 13:1O:58:LEU:HD11  | 13:1O:86:LEU:HD22  | 1.81                     | 0.62              |
| 35:1a:783:C:OP1    | 35:1a:1515:G:O2'   | 2.17                     | 0.62              |
| 47:1m:7:ASN:HD22   | 47:1m:21:ILE:HD11  | 1.64                     | 0.62              |
| 1:1A:1905:C:N4     | 1:1A:1969:A:OP2    | 2.32                     | 0.61              |
| 22:1X:3:ARG:HH12   | 22:1X:7:LEU:HD21   | 1.64                     | 0.61              |
| 35:1a:362:G:N2     | 35:1a:365:U:OP2    | 2.23                     | 0.61              |
| 39:1e:14:LEU:HA    | 39:1e:36:THR:HG22  | 1.80                     | 0.61              |
| 1:1A:2357:G:N2     | 1:1A:2360:G:OP2    | 2.24                     | 0.61              |
| 11:1K:11:GLN:NE2   | 11:1K:54:ILE:O     | 2.33                     | 0.61              |
| 12:1N:17:VAL:HG23  | 12:1N:137:PRO:HB2  | 1.82                     | 0.61              |
| 41:1g:12:LEU:HD12  | 41:1g:13:PRO:HD2   | 1.82                     | 0.61              |
| 49:1o:35:ILE:HG23  | 49:1o:55:LEU:HD11  | 1.81                     | 0.61              |
| 1:1A:1800:C:OP1    | 3:1D:257:ARG:NH2   | 2.33                     | 0.61              |
| 41:1g:112:ASP:H    | 41:1g:118:ARG:HD3  | 1.64                     | 0.61              |
| 1:1A:987:C:O2'     | 1:1A:1000:A:N3     | 2.32                     | 0.61              |
| 1:1A:2853:C:H2'    | 1:1A:2854:G:H8     | 1.65                     | 0.61              |
| 14:1P:33:ARG:NH2   | 14:1P:39:LYS:O     | 2.32                     | 0.61              |
| 1:1A:527:C:N4      | 1:1A:2777:G:O2'    | 2.33                     | 0.61              |
| 35:1a:1385:G:H2'   | 35:1a:1386:G:H8    | 1.65                     | 0.61              |
| 1:1A:451:U:O2      | 1:1A:453:A:N6      | 2.32                     | 0.61              |
| 16:1R:79:LEU:HD23  | 16:1R:83:LEU:HD12  | 1.83                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:1a:362:G:OP1   | 46:1l:57:THR:OG1  | 2.19                     | 0.61              |
| 35:1a:1347:G:O2'  | 35:1a:1348:U:O5'  | 2.19                     | 0.61              |
| 1:1A:499:U:H5''   | 23:1Y:42:LYS:HE2  | 1.81                     | 0.61              |
| 9:1I:28:ASN:OD1   | 26:11:35:HIS:NE2  | 2.30                     | 0.61              |
| 35:1a:9:G:H5'     | 39:1e:107:GLY:HA3 | 1.81                     | 0.61              |
| 1:1A:1341:G:OP1   | 1:1A:1602:U:O2'   | 2.18                     | 0.61              |
| 35:1a:166:U:H2'   | 35:1a:167:A:H8    | 1.64                     | 0.61              |
| 1:1A:1363:C:O2'   | 1:1A:1809:A:N3    | 2.34                     | 0.61              |
| 41:1g:67:ASN:O    | 41:1g:137:ARG:NE  | 2.33                     | 0.61              |
| 45:1k:22:ILE:HG12 | 45:1k:31:VAL:HG13 | 1.83                     | 0.61              |
| 22:1X:14:PRO:HD3  | 27:12:30:MET:HG3  | 1.83                     | 0.61              |
| 24:1Z:86:LEU:HD13 | 24:1Z:89:ILE:HD11 | 1.81                     | 0.61              |
| 35:1a:273:U:O4    | 35:1a:274:A:N6    | 2.33                     | 0.60              |
| 35:1a:1345:U:H1'  | 35:1a:1375:A:H61  | 1.64                     | 0.60              |
| 54:1t:70:LYS:HG3  | 54:1t:73:ARG:HH22 | 1.66                     | 0.60              |
| 1:1A:772:C:O2     | 3:1D:42:ARG:NH1   | 2.35                     | 0.60              |
| 10:1J:88:HIS:HB2  | 10:1J:89:PRO:HD3  | 1.83                     | 0.60              |
| 1:1A:605:G:OP1    | 5:1F:99:LYS:NZ    | 2.34                     | 0.60              |
| 1:1A:1912:A:O2'   | 35:1a:1494:G:O2'  | 2.18                     | 0.60              |
| 6:1G:97:GLU:OE2   | 29:14:25:ARG:N    | 2.31                     | 0.60              |
| 33:18:32:LEU:HB3  | 33:18:40:LYS:HD3  | 1.82                     | 0.60              |
| 43:1i:12:LYS:O    | 43:1i:14:SER:N    | 2.32                     | 0.60              |
| 1:1A:581:C:H2'    | 1:1A:582:A:C8     | 2.37                     | 0.60              |
| 4:1E:110:THR:O    | 4:1E:202:ILE:N    | 2.23                     | 0.60              |
| 35:1a:1121:U:H3   | 35:1a:1152:A:H61  | 1.49                     | 0.60              |
| 36:1b:166:ASP:HB2 | 36:1b:190:SER:HA  | 1.83                     | 0.60              |
| 1:1A:594:U:H2'    | 1:1A:595:C:C6     | 2.36                     | 0.60              |
| 1:1A:1765:U:H2'   | 1:1A:1766:G:H8    | 1.65                     | 0.60              |
| 1:1A:1998:A:OP2   | 4:1E:141:ARG:NH1  | 2.34                     | 0.60              |
| 1:1A:2591:C:H2'   | 1:1A:2592:G:C8    | 2.37                     | 0.60              |
| 1:1A:2831:G:OP2   | 4:1E:59:ARG:NH1   | 2.33                     | 0.60              |
| 1:1A:2420:C:H2'   | 1:1A:2421:G:C8    | 2.36                     | 0.60              |
| 9:1I:124:THR:O    | 9:1I:128:HIS:NE2  | 2.32                     | 0.60              |
| 24:1Z:25:LYS:HG2  | 24:1Z:43:ASP:HA   | 1.82                     | 0.60              |
| 36:1b:92:ASN:OD1  | 36:1b:93:HIS:ND1  | 2.35                     | 0.60              |
| 1:1A:2788:C:O2'   | 1:1A:2809:A:N3    | 2.32                     | 0.60              |
| 35:1a:28:A:O2'    | 35:1a:296:U:OP1   | 2.16                     | 0.60              |
| 1:1A:789:A:H5'    | 32:17:4:THR:HG21  | 1.82                     | 0.60              |
| 1:1A:1615:C:OP2   | 1:1A:1617:C:N4    | 2.35                     | 0.60              |
| 1:1A:2101:A:H2'   | 1:1A:2102:G:H8    | 1.66                     | 0.60              |
| 27:12:24:GLU:HB3  | 27:12:46:VAL:HG21 | 1.83                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:16:3:GLY:O     | 31:16:5:ARG:N      | 2.33                     | 0.60              |
| 35:1a:719:C:H42   | 52:1r:59:LYS:HE2   | 1.67                     | 0.60              |
| 35:1a:749:A:O2'   | 49:1o:19:ASN:OD1   | 2.19                     | 0.60              |
| 35:1a:1237:C:OP1  | 35:1a:1303:C:O2'   | 2.18                     | 0.60              |
| 47:1m:24:VAL:HG23 | 47:1m:28:ARG:HB3   | 1.84                     | 0.60              |
| 21:1W:56:ALA:HA   | 21:1W:59:GLU:HG2   | 1.82                     | 0.60              |
| 45:1k:88:PRO:HA   | 45:1k:92:ARG:HD2   | 1.83                     | 0.60              |
| 1:1A:834:G:O2'    | 1:1A:2358:A:O2'    | 2.10                     | 0.60              |
| 17:1S:33:ARG:HG2  | 17:1S:34:HIS:CD2   | 2.37                     | 0.60              |
| 4:1E:130:GLN:OE1  | 4:1E:139:SER:OG    | 2.20                     | 0.59              |
| 18:1T:52:ARG:H    | 18:1T:56:SER:HB3   | 1.68                     | 0.59              |
| 45:1k:24:ALA:HA   | 45:1k:29:THR:HA    | 1.83                     | 0.59              |
| 1:1A:2420:C:H5''  | 31:16:7:LYS:HD2    | 1.84                     | 0.59              |
| 5:1F:75:SER:HB3   | 5:1F:78:TRP:CD1    | 2.36                     | 0.59              |
| 1:1A:269:C:H2'    | 1:1A:270:A:H8      | 1.66                     | 0.59              |
| 1:1A:563:A:N3     | 19:1U:36:GLN:NE2   | 2.49                     | 0.59              |
| 1:1A:1818:U:H5'   | 3:1D:156:SER:HB2   | 1.85                     | 0.59              |
| 31:16:36:LYS:HG3  | 31:16:47:ILE:HG13  | 1.82                     | 0.59              |
| 45:1k:22:ILE:O    | 45:1k:86:LYS:N     | 2.35                     | 0.59              |
| 1:1A:69:C:O2      | 1:1A:73:A:O2'      | 2.18                     | 0.59              |
| 1:1A:1660:G:H2'   | 1:1A:1661:G:H8     | 1.67                     | 0.59              |
| 2:1B:28:C:H2'     | 2:1B:29:A:C8       | 2.37                     | 0.59              |
| 3:1D:56:GLY:HA2   | 3:1D:212:TRP:HA    | 1.83                     | 0.59              |
| 35:1a:257:G:H2'   | 35:1a:258:G:H8     | 1.67                     | 0.59              |
| 35:1a:1400:C:H5'  | 58:1x:34:G:H1      | 1.68                     | 0.59              |
| 53:1s:62:THR:HG22 | 53:1s:63:ASP:H     | 1.66                     | 0.59              |
| 1:1A:30:G:O2'     | 1:1A:1214:A:N3     | 2.35                     | 0.59              |
| 1:1A:1310:G:H1'   | 1:1A:1611:C:H5''   | 1.84                     | 0.59              |
| 6:1G:35:LEU:HB2   | 6:1G:88:VAL:HB     | 1.85                     | 0.59              |
| 37:1c:109:GLU:HB2 | 37:1c:143:LEU:HD13 | 1.84                     | 0.59              |
| 41:1g:87:PRO:HG3  | 41:1g:148:LYS:HA   | 1.84                     | 0.59              |
| 1:1A:1062:G:N2    | 11:1K:134:SER:OG   | 2.35                     | 0.59              |
| 1:1A:2033:A:O2'   | 1:1A:2035:G:OP1    | 2.18                     | 0.59              |
| 1:1A:2444:G:H2'   | 1:1A:2445:2MG:O4'  | 2.02                     | 0.59              |
| 24:1Z:77:VAL:HG23 | 24:1Z:89:ILE:HG12  | 1.84                     | 0.59              |
| 27:12:16:THR:O    | 27:12:20:ASN:ND2   | 2.34                     | 0.59              |
| 35:1a:1352:C:H2'  | 35:1a:1353:G:C8    | 2.38                     | 0.59              |
| 1:1A:1031:G:H2'   | 1:1A:1032:A:C8     | 2.37                     | 0.59              |
| 1:1A:1031:G:H2'   | 1:1A:1032:A:H8     | 1.68                     | 0.59              |
| 1:1A:2528:U:O2'   | 1:1A:2530:A:OP1    | 2.18                     | 0.59              |
| 26:11:39:VAL:HG12 | 26:11:42:GLU:H     | 1.68                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:955:PSU:H5'   | 15:1Q:86:LYS:HD3  | 1.84                     | 0.59              |
| 1:1A:2431:U:N3     | 1:1A:2434:A:OP2   | 2.26                     | 0.59              |
| 37:1c:91:ALA:HA    | 37:1c:94:ALA:HB3  | 1.85                     | 0.59              |
| 1:1A:1528:A:N6     | 1:1A:1543:G:O2'   | 2.36                     | 0.59              |
| 6:1G:28:PRO:HB2    | 6:1G:168:LEU:HD22 | 1.85                     | 0.59              |
| 14:1P:29:LYS:HG2   | 14:1P:30:THR:HG23 | 1.84                     | 0.59              |
| 42:1h:76:ARG:NH2   | 42:1h:78:SER:O    | 2.36                     | 0.59              |
| 43:1i:19:PHE:HB2   | 43:1i:63:TYR:HB3  | 1.84                     | 0.59              |
| 11:1K:44:LYS:HE2   | 11:1K:70:THR:HG21 | 1.85                     | 0.58              |
| 35:1a:1308:U:H2'   | 35:1a:1309:G:H8   | 1.68                     | 0.58              |
| 35:1a:1524:C:H2'   | 35:1a:1525:G:H8   | 1.68                     | 0.58              |
| 39:1e:73:VAL:HG11  | 39:1e:143:LEU:HB3 | 1.83                     | 0.58              |
| 47:1m:15:VAL:HG23  | 47:1m:16:ILE:HD12 | 1.83                     | 0.58              |
| 49:1o:77:TYR:OH    | 49:1o:87:ARG:NH2  | 2.35                     | 0.58              |
| 1:1A:931:U:O2      | 1:1A:1167:C:O2'   | 2.16                     | 0.58              |
| 1:1A:1022:G:H4'    | 1:1A:1023:U:O5'   | 2.03                     | 0.58              |
| 37:1c:20:THR:HB    | 37:1c:57:GLU:HG2  | 1.84                     | 0.58              |
| 38:1d:172:VAL:HG22 | 38:1d:174:ALA:H   | 1.66                     | 0.58              |
| 1:1A:1423:G:H2'    | 1:1A:1424:G:C8    | 2.38                     | 0.58              |
| 1:1A:1801:A:N6     | 1:1A:2201:G:O2'   | 2.36                     | 0.58              |
| 1:1A:2260:C:N4     | 25:10:10:ARG:HD2  | 2.17                     | 0.58              |
| 51:1q:12:VAL:HB    | 51:1q:21:VAL:HG13 | 1.85                     | 0.58              |
| 10:1J:103:ASN:HA   | 10:1J:107:GLU:HB3 | 1.83                     | 0.58              |
| 23:1Y:40:LEU:HD23  | 23:1Y:61:GLU:HG3  | 1.84                     | 0.58              |
| 35:1a:1502:A:N7    | 35:1a:1505:G:N2   | 2.51                     | 0.58              |
| 46:1l:51:VAL:HG23  | 46:1l:65:TYR:HA   | 1.85                     | 0.58              |
| 53:1s:40:PHE:HB2   | 53:1s:43:MET:HG3  | 1.84                     | 0.58              |
| 1:1A:2339:C:H2'    | 1:1A:2340:A:C8    | 2.39                     | 0.58              |
| 35:1a:1187:G:H5'   | 43:1i:114:LYS:HE3 | 1.86                     | 0.58              |
| 36:1b:19:THR:OG1   | 36:1b:20:ARG:N    | 2.35                     | 0.58              |
| 6:1G:1:ALA:N       | 6:1G:100:GLU:OE1  | 2.36                     | 0.58              |
| 6:1G:62:GLN:HE22   | 6:1G:90:LEU:HB3   | 1.69                     | 0.58              |
| 35:1a:311:C:OP1    | 50:1p:31:ARG:NH1  | 2.37                     | 0.58              |
| 1:1A:1323:C:OP1    | 21:1W:98:LYS:NZ   | 2.37                     | 0.58              |
| 35:1a:377:G:H5''   | 50:1p:24:SER:HB2  | 1.86                     | 0.58              |
| 37:1c:106:ARG:HG3  | 37:1c:107:LYS:HG3 | 1.84                     | 0.58              |
| 37:1c:190:THR:OG1  | 37:1c:193:GLY:O   | 2.22                     | 0.58              |
| 45:1k:21:HIS:HA    | 45:1k:84:MET:HB2  | 1.86                     | 0.58              |
| 1:1A:2346:A:O2'    | 31:16:37:LYS:NZ   | 2.37                     | 0.58              |
| 35:1a:897:C:H2'    | 35:1a:898:G:H8    | 1.69                     | 0.58              |
| 44:1j:59:LYS:HE2   | 44:1j:62:ARG:HH21 | 1.69                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2200:C:OP1   | 26:11:36:ARG:N     | 2.33                     | 0.57              |
| 6:1G:104:THR:HG21 | 29:14:22:MET:HE1   | 1.84                     | 0.57              |
| 35:1a:923:A:OP1   | 39:1e:25:LYS:NZ    | 2.28                     | 0.57              |
| 41:1g:91:ARG:O    | 41:1g:95:ARG:N     | 2.37                     | 0.57              |
| 14:1P:96:LYS:HD3  | 14:1P:103:ILE:HA   | 1.85                     | 0.57              |
| 35:1a:758:C:H4'   | 35:1a:880:C:H4'    | 1.86                     | 0.57              |
| 1:1A:575:A:OP2    | 1:1A:2499:C:O2'    | 2.21                     | 0.57              |
| 1:1A:2189:U:H2'   | 1:1A:2190:G:C8     | 2.40                     | 0.57              |
| 35:1a:1068:G:OP1  | 35:1a:1387:G:O2'   | 2.22                     | 0.57              |
| 1:1A:698:C:OP1    | 1:1A:1634:A:N6     | 2.21                     | 0.57              |
| 1:1A:2260:C:H42   | 25:10:10:ARG:HD2   | 1.68                     | 0.57              |
| 21:1W:29:VAL:HG22 | 21:1W:71:VAL:HG23  | 1.85                     | 0.57              |
| 35:1a:235:C:H2'   | 35:1a:236:A:H8     | 1.68                     | 0.57              |
| 21:1W:29:VAL:HG21 | 21:1W:69:LEU:HG    | 1.87                     | 0.57              |
| 37:1c:171:ARG:HG2 | 37:1c:173:PRO:HD3  | 1.85                     | 0.57              |
| 1:1A:1765:U:H2'   | 1:1A:1766:G:C8     | 2.39                     | 0.57              |
| 1:1A:2508:G:H2'   | 1:1A:2509:G:H8     | 1.70                     | 0.57              |
| 4:1E:15:PHE:H     | 18:1T:11:GLN:NE2   | 2.02                     | 0.57              |
| 42:1h:103:VAL:HB  | 42:1h:124:ILE:HG22 | 1.86                     | 0.57              |
| 5:1F:88:ARG:O     | 5:1F:90:GLN:N      | 2.37                     | 0.57              |
| 27:12:2:LYS:HB3   | 27:12:52:ARG:HD3   | 1.86                     | 0.57              |
| 52:1r:62:ARG:HD3  | 52:1r:69:TYR:CD1   | 2.40                     | 0.57              |
| 1:1A:1469:A:H2'   | 1:1A:1470:A:C8     | 2.39                     | 0.57              |
| 4:1E:46:ARG:NH2   | 4:1E:89:GLU:OE1    | 2.37                     | 0.57              |
| 35:1a:1323:G:H2'  | 35:1a:1324:A:C8    | 2.40                     | 0.57              |
| 40:1f:5:GLU:HA    | 40:1f:63:ASN:HA    | 1.85                     | 0.57              |
| 1:1A:1352:U:O2'   | 1:1A:1570:A:N3     | 2.34                     | 0.57              |
| 1:1A:2283:C:OP1   | 31:16:3:GLY:N      | 2.38                     | 0.57              |
| 4:1E:156:PHE:HB3  | 12:1N:81:ILE:HG13  | 1.87                     | 0.57              |
| 6:1G:7:TYR:OH     | 6:1G:28:PRO:O      | 2.23                     | 0.57              |
| 6:1G:141:ASP:HB2  | 6:1G:144:LYS:HD3   | 1.87                     | 0.57              |
| 14:1P:62:PRO:HD3  | 33:18:26:ALA:HB2   | 1.85                     | 0.57              |
| 26:11:16:ASN:N    | 26:11:24:THR:O     | 2.36                     | 0.57              |
| 35:1a:522:C:N4    | 46:1l:49:ARG:HH22  | 2.03                     | 0.57              |
| 35:1a:1027:C:N4   | 35:1a:1035:A:N1    | 2.44                     | 0.57              |
| 43:1i:11:ARG:HA   | 43:1i:105:ARG:HH12 | 1.69                     | 0.57              |
| 51:1q:21:VAL:HA   | 51:1q:44:HIS:HA    | 1.86                     | 0.57              |
| 39:1e:37:VAL:HG22 | 39:1e:47:PHE:HA    | 1.86                     | 0.57              |
| 1:1A:2743:U:O2'   | 7:1H:152:ARG:NH1   | 2.38                     | 0.56              |
| 35:1a:589:U:H5''  | 42:1h:29:SER:HB2   | 1.87                     | 0.56              |
| 35:1a:828:U:H2'   | 36:1b:24:PRO:HB3   | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:444:C:OP2    | 5:1F:44:ARG:NH2   | 2.38                     | 0.56              |
| 1:1A:1154:G:OP2   | 19:1U:57:ARG:NH1  | 2.36                     | 0.56              |
| 3:1D:41:GLY:O     | 3:1D:49:THR:OG1   | 2.20                     | 0.56              |
| 1:1A:463:G:N2     | 1:1A:465:G:H3'    | 2.21                     | 0.56              |
| 1:1A:647:G:N2     | 1:1A:2350:C:O2'   | 2.38                     | 0.56              |
| 1:1A:1296:G:OP1   | 1:1A:2709:G:O2'   | 2.21                     | 0.56              |
| 1:1A:1818:U:C5    | 3:1D:155:ARG:HD3  | 2.40                     | 0.56              |
| 15:1Q:49:ALA:O    | 15:1Q:53:MET:HG2  | 2.06                     | 0.56              |
| 18:1T:70:GLU:OE2  | 18:1T:100:ARG:NH1 | 2.38                     | 0.56              |
| 35:1a:421:U:O2'   | 35:1a:422:C:OP1   | 2.23                     | 0.56              |
| 35:1a:578:C:O2'   | 35:1a:728:A:N3    | 2.32                     | 0.56              |
| 1:1A:742:A:H2'    | 1:1A:743:A:C8     | 2.41                     | 0.56              |
| 1:1A:970:U:H2'    | 1:1A:971:G:H8     | 1.70                     | 0.56              |
| 1:1A:2853:C:H2'   | 1:1A:2854:G:C8    | 2.39                     | 0.56              |
| 11:1K:38:CYS:O    | 11:1K:42:ASN:ND2  | 2.34                     | 0.56              |
| 35:1a:8:A:N6      | 38:1d:201:GLU:O   | 2.38                     | 0.56              |
| 1:1A:197:A:H4'    | 1:1A:2069:G7M:OP2 | 2.05                     | 0.56              |
| 1:1A:1820:U:H5    | 3:1D:176:ARG:HH21 | 1.53                     | 0.56              |
| 3:1D:137:GLY:H    | 3:1D:163:ILE:HB   | 1.69                     | 0.56              |
| 20:1V:31:GLU:HG3  | 20:1V:32:THR:H    | 1.71                     | 0.56              |
| 35:1a:1287:A:H2   | 35:1a:1353:G:H1'  | 1.71                     | 0.56              |
| 37:1c:54:ILE:HD12 | 37:1c:56:ILE:HD11 | 1.87                     | 0.56              |
| 44:1j:57:VAL:HG22 | 44:1j:58:ASN:H    | 1.69                     | 0.56              |
| 1:1A:546:U:H2'    | 1:1A:547:A:H4'    | 1.87                     | 0.56              |
| 1:1A:2030:6MZ:N3  | 1:1A:2499:C:H5''  | 2.20                     | 0.56              |
| 1:1A:2443:C:H2'   | 1:1A:2444:G:C8    | 2.40                     | 0.56              |
| 13:1O:8:LEU:HB2   | 13:1O:19:VAL:HG23 | 1.88                     | 0.56              |
| 20:1V:61:ALA:HB1  | 20:1V:96:VAL:HB   | 1.87                     | 0.56              |
| 40:1f:46:GLN:HA   | 40:1f:56:LYS:HG2  | 1.87                     | 0.56              |
| 43:1i:24:ASN:OD1  | 43:1i:25:GLY:N    | 2.38                     | 0.56              |
| 44:1j:54:SER:OG   | 44:1j:57:VAL:O    | 2.19                     | 0.56              |
| 46:1l:45:ASN:ND2  | 46:1l:88:ASP:OD1  | 2.38                     | 0.56              |
| 5:1F:7:ASP:OD1    | 5:1F:8:ALA:N      | 2.36                     | 0.56              |
| 35:1a:257:G:H1    | 35:1a:269:C:H42   | 1.54                     | 0.56              |
| 35:1a:355:C:H1'   | 35:1a:388:G:H1'   | 1.88                     | 0.56              |
| 1:1A:878:A:H3'    | 1:1A:879:G:H8     | 1.71                     | 0.56              |
| 1:1A:1799:G:O5'   | 1:1A:1819:A:N6    | 2.39                     | 0.56              |
| 10:1J:44:ALA:HB2  | 10:1J:52:MET:HE2  | 1.88                     | 0.56              |
| 33:18:28:LEU:HA   | 33:18:32:LEU:HD21 | 1.87                     | 0.56              |
| 35:1a:572:A:H5''  | 35:1a:917:G:H4'   | 1.86                     | 0.56              |
| 35:1a:950:U:H2'   | 35:1a:951:G:H8    | 1.71                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:774:G:H1'     | 1:1A:777:G:H21     | 1.69                     | 0.56              |
| 1:1A:2087:G:H2'    | 1:1A:2088:A:C8     | 2.41                     | 0.56              |
| 1:1A:2399:G:N2     | 1:1A:2417:C:N3     | 2.52                     | 0.56              |
| 3:1D:171:VAL:N     | 3:1D:183:VAL:O     | 2.38                     | 0.56              |
| 44:1j:52:LEU:HD23  | 44:1j:62:ARG:HG2   | 1.87                     | 0.56              |
| 1:1A:558:U:H2'     | 1:1A:559:G:H8      | 1.72                     | 0.55              |
| 10:1J:48:ALA:HB3   | 10:1J:51:TYR:HE2   | 1.71                     | 0.55              |
| 35:1a:959:A:HO2'   | 35:1a:984:C:HO2'   | 1.48                     | 0.55              |
| 38:1d:131:ILE:HG22 | 38:1d:133:SER:H    | 1.70                     | 0.55              |
| 45:1k:111:ASP:O    | 52:1r:72:ARG:NH2   | 2.39                     | 0.55              |
| 1:1A:247:G:O2'     | 1:1A:386:G:N1      | 2.40                     | 0.55              |
| 1:1A:2391:G:O2'    | 1:1A:2392:A:O5'    | 2.20                     | 0.55              |
| 1:1A:2893:A:H5''   | 1:1A:2894:G:H5'    | 1.87                     | 0.55              |
| 3:1D:153:LEU:HD11  | 3:1D:181:ARG:NH2   | 2.21                     | 0.55              |
| 35:1a:1516:2MG:C2  | 35:1a:1520:C:N3    | 2.75                     | 0.55              |
| 38:1d:187:ARG:HH12 | 38:1d:192:ALA:H    | 1.54                     | 0.55              |
| 43:1i:56:MET:O     | 43:1i:58:GLU:N     | 2.39                     | 0.55              |
| 48:1n:89:MET:HE1   | 48:1n:98:LYS:HD2   | 1.88                     | 0.55              |
| 1:1A:694:U:H3      | 1:1A:768:G:H1      | 1.53                     | 0.55              |
| 1:1A:771:G:OP2     | 32:17:11:LYS:NZ    | 2.40                     | 0.55              |
| 1:1A:2529:G:H4'    | 7:1H:174:LYS:HG3   | 1.88                     | 0.55              |
| 41:1g:115:MET:HB2  | 41:1g:118:ARG:HH21 | 1.71                     | 0.55              |
| 45:1k:36:ARG:NH1   | 45:1k:82:GLU:OE2   | 2.36                     | 0.55              |
| 1:1A:1309:G:HO2'   | 1:1A:1611:C:HO2'   | 1.52                     | 0.55              |
| 1:1A:1826:G:O2'    | 1:1A:1971:U:OP2    | 2.18                     | 0.55              |
| 1:1A:2830:C:O2'    | 1:1A:2883:A:N1     | 2.37                     | 0.55              |
| 3:1D:204:LEU:HD22  | 3:1D:209:ALA:HB1   | 1.87                     | 0.55              |
| 30:15:27:LEU:HD23  | 30:15:36:LYS:HB3   | 1.88                     | 0.55              |
| 35:1a:54:C:H2'     | 35:1a:352:C:H41    | 1.72                     | 0.55              |
| 35:1a:337:G:H2'    | 35:1a:338:A:C8     | 2.41                     | 0.55              |
| 36:1b:202:ASN:OD1  | 36:1b:203:ASP:N    | 2.40                     | 0.55              |
| 58:1x:64:C:H2'     | 58:1x:65:PSU:C6    | 2.42                     | 0.55              |
| 1:1A:1796:U:H2'    | 1:1A:1797:G:C8     | 2.40                     | 0.55              |
| 1:1A:599:A:H2'     | 1:1A:600:G:H8      | 1.71                     | 0.55              |
| 1:1A:1844:C:H2'    | 1:1A:1845:G:H8     | 1.71                     | 0.55              |
| 1:1A:2461:A:N6     | 1:1A:2488:G:O6     | 2.40                     | 0.55              |
| 4:1E:47:ALA:HA     | 4:1E:84:LEU:HG     | 1.88                     | 0.55              |
| 35:1a:1385:G:H2'   | 35:1a:1386:G:C8    | 2.42                     | 0.55              |
| 35:1a:1485:U:H2'   | 35:1a:1486:G:H8    | 1.72                     | 0.55              |
| 35:1a:1497:G:H2'   | 35:1a:1498:UR3:H5' | 1.87                     | 0.55              |
| 44:1j:7:ARG:HB3    | 44:1j:101:SER:HB2  | 1.89                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:690:G:N2     | 1:1A:772:C:N3      | 2.54                     | 0.55              |
| 1:1A:2075:U:OP2   | 1:1A:2238:G:O2'    | 2.24                     | 0.55              |
| 33:18:22:LYS:HB2  | 33:18:46:LYS:HB3   | 1.87                     | 0.55              |
| 35:1a:1053:G:H4'  | 35:1a:1054:C:H3'   | 1.89                     | 0.55              |
| 1:1A:676:A:H62    | 1:1A:802:A:H61     | 1.55                     | 0.55              |
| 1:1A:1514:G:O2'   | 1:1A:1557:C:O2'    | 2.24                     | 0.55              |
| 1:1A:2260:C:O2'   | 1:1A:2388:A:O2'    | 2.25                     | 0.55              |
| 16:1R:51:LEU:HD21 | 16:1R:69:ARG:HD2   | 1.89                     | 0.55              |
| 23:1Y:52:ASN:OD1  | 23:1Y:53:GLN:N     | 2.40                     | 0.55              |
| 35:1a:166:U:H2'   | 35:1a:167:A:C8     | 2.42                     | 0.55              |
| 35:1a:504:C:H2'   | 35:1a:511:C:H5     | 1.71                     | 0.55              |
| 35:1a:958:A:C2    | 53:1s:54:ARG:HB3   | 2.41                     | 0.55              |
| 38:1d:185:PRO:HB2 | 38:1d:190:LEU:HD23 | 1.89                     | 0.55              |
| 1:1A:2198:A:C2    | 9:1I:29:PHE:HB2    | 2.42                     | 0.55              |
| 10:1J:53:ARG:HB3  | 10:1J:55:VAL:HG13  | 1.89                     | 0.55              |
| 14:1P:33:ARG:HD2  | 14:1P:40:SER:HA    | 1.89                     | 0.55              |
| 15:1Q:69:PRO:HA   | 15:1Q:94:ALA:HB2   | 1.88                     | 0.55              |
| 31:16:18:HIS:HE1  | 31:16:20:TYR:CZ    | 2.25                     | 0.55              |
| 50:1p:43:ALA:HB1  | 50:1p:46:LYS:HE3   | 1.88                     | 0.55              |
| 1:1A:75:G:OP1     | 27:12:48:ARG:NH2   | 2.40                     | 0.54              |
| 1:1A:290:U:H2'    | 1:1A:291:G:H8      | 1.72                     | 0.54              |
| 1:1A:538:A:H4'    | 12:1N:7:LYS:HG2    | 1.89                     | 0.54              |
| 1:1A:827:U:O2'    | 1:1A:2068:U:O2     | 2.26                     | 0.54              |
| 3:1D:180:MET:HB2  | 3:1D:267:VAL:HB    | 1.89                     | 0.54              |
| 35:1a:195:A:N3    | 35:1a:222:C:O2'    | 2.38                     | 0.54              |
| 35:1a:753:A:H5'   | 35:1a:754:C:C5     | 2.41                     | 0.54              |
| 42:1h:73:SER:OG   | 42:1h:75:GLN:NE2   | 2.40                     | 0.54              |
| 55:1u:36:PHE:HB3  | 55:1u:40:PRO:HD3   | 1.89                     | 0.54              |
| 1:1A:247:G:HO2'   | 1:1A:386:G:H1      | 1.52                     | 0.54              |
| 1:1A:351:C:H2'    | 1:1A:352:A:C8      | 2.42                     | 0.54              |
| 1:1A:2027:G:H1    | 1:1A:2036:C:H42    | 1.56                     | 0.54              |
| 3:1D:184:GLU:HB3  | 3:1D:187:CYS:SG    | 2.47                     | 0.54              |
| 6:1G:64:PRO:HB3   | 6:1G:88:VAL:HG22   | 1.90                     | 0.54              |
| 35:1a:1503:A:OP1  | 35:1a:1531:A:O2'   | 2.19                     | 0.54              |
| 39:1e:110:MET:HG3 | 39:1e:139:THR:HG21 | 1.88                     | 0.54              |
| 1:1A:177:G:OP2    | 1:1A:177:G:N2      | 2.30                     | 0.54              |
| 3:1D:106:PRO:HG2  | 3:1D:109:LEU:HB2   | 1.88                     | 0.54              |
| 35:1a:801:U:H2'   | 35:1a:802:A:C8     | 2.41                     | 0.54              |
| 1:1A:321:U:H5''   | 5:1F:131:THR:HG23  | 1.89                     | 0.54              |
| 1:1A:783:A:H2'    | 1:1A:784:G:H4'     | 1.89                     | 0.54              |
| 1:1A:1261:C:OP2   | 21:1W:83:LYS:NZ    | 2.31                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2748:A:H5'    | 7:1H:3:VAL:HG21    | 1.88                     | 0.54              |
| 6:1G:147:ARG:HG3   | 6:1G:149:ARG:H     | 1.72                     | 0.54              |
| 20:1V:69:GLY:N     | 20:1V:91:GLN:O     | 2.34                     | 0.54              |
| 35:1a:1100:C:N4    | 35:1a:1103:C:OP1   | 2.40                     | 0.54              |
| 38:1d:151:GLN:O    | 38:1d:153:ARG:N    | 2.40                     | 0.54              |
| 1:1A:434:U:O2'     | 1:1A:436:C:N4      | 2.40                     | 0.54              |
| 1:1A:2744:G:N2     | 7:1H:142:GLN:OE1   | 2.34                     | 0.54              |
| 35:1a:987:G:H2'    | 35:1a:988:G:H8     | 1.73                     | 0.54              |
| 35:1a:1053:G:N2    | 35:1a:1058:G:O6    | 2.41                     | 0.54              |
| 35:1a:1513:A:H2'   | 35:1a:1514:G:C8    | 2.42                     | 0.54              |
| 55:1u:64:ALA:O     | 55:1u:66:ARG:N     | 2.40                     | 0.54              |
| 1:1A:586:A:N1      | 1:1A:809:G:O2'     | 2.37                     | 0.54              |
| 1:1A:674:G:H5''    | 5:1F:71:GLY:N      | 2.21                     | 0.54              |
| 1:1A:939:G:H2'     | 1:1A:940:G:H8      | 1.72                     | 0.54              |
| 1:1A:2282:G:N2     | 1:1A:2390:U:O2     | 2.39                     | 0.54              |
| 2:1B:29:A:O2'      | 2:1B:58:A:N1       | 2.37                     | 0.54              |
| 21:1W:83:LYS:O     | 21:1W:84:ARG:NH2   | 2.37                     | 0.54              |
| 35:1a:490:C:OP1    | 38:1d:145:ARG:NH2  | 2.30                     | 0.54              |
| 39:1e:44:ARG:HH22  | 39:1e:70:MET:HE3   | 1.72                     | 0.54              |
| 45:1k:59:PRO:HD3   | 45:1k:90:PRO:HB2   | 1.89                     | 0.54              |
| 1:1A:144:A:H4'     | 22:1X:2:ILE:HD11   | 1.90                     | 0.54              |
| 1:1A:1013:C:H2'    | 1:1A:1014:A:H8     | 1.72                     | 0.54              |
| 1:1A:2224:G:H4'    | 1:1A:2226:C:C2     | 2.43                     | 0.54              |
| 12:1N:40:HIS:CE1   | 12:1N:41:LYS:HG3   | 2.42                     | 0.54              |
| 27:12:26:PHE:HD1   | 27:12:29:ARG:HH11  | 1.56                     | 0.54              |
| 35:1a:77:A:H2'     | 35:1a:78:A:C8      | 2.42                     | 0.54              |
| 42:1h:17:GLN:NE2   | 42:1h:69:ALA:HB1   | 2.23                     | 0.54              |
| 43:1i:18:VAL:HG13  | 43:1i:64:ILE:HG12  | 1.88                     | 0.54              |
| 1:1A:351:C:H2'     | 1:1A:352:A:H8      | 1.72                     | 0.54              |
| 1:1A:715:A:H61     | 49:1o:52:ARG:NH1   | 2.06                     | 0.54              |
| 1:1A:1012:U:O2     | 12:1N:27:ARG:NH1   | 2.40                     | 0.54              |
| 1:1A:1028:A:N6     | 1:1A:1125:G:H2'    | 2.22                     | 0.54              |
| 12:1N:56:VAL:HB    | 12:1N:124:VAL:HG12 | 1.89                     | 0.54              |
| 37:1c:13:ILE:HG22  | 37:1c:14:VAL:HG23  | 1.89                     | 0.54              |
| 42:1h:100:ILE:HD13 | 42:1h:111:THR:HG22 | 1.90                     | 0.54              |
| 50:1p:5:ARG:NH2    | 50:1p:26:ASN:O     | 2.31                     | 0.54              |
| 1:1A:1094:U:N3     | 1:1A:1097:U:OP2    | 2.35                     | 0.54              |
| 12:1N:35:ARG:HB2   | 12:1N:54:ILE:HD11  | 1.90                     | 0.54              |
| 35:1a:701:U:OP1    | 35:1a:702:A:O2'    | 2.13                     | 0.54              |
| 35:1a:897:C:H2'    | 35:1a:898:G:C8     | 2.42                     | 0.54              |
| 7:1H:88:LEU:HD23   | 7:1H:93:TYR:HB3    | 1.90                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:1a:12:U:H4'    | 35:1a:526:C:H4'    | 1.90                     | 0.54              |
| 35:1a:119:A:OP2   | 35:1a:288:A:N6     | 2.41                     | 0.54              |
| 35:1a:1368:A:H5'' | 48:1n:101:TRP:HZ2  | 1.72                     | 0.54              |
| 1:1A:4:U:H2'      | 1:1A:5:A:H8        | 1.73                     | 0.53              |
| 1:1A:690:G:H21    | 3:1D:42:ARG:HH12   | 1.55                     | 0.53              |
| 15:1Q:21:ALA:HB1  | 15:1Q:100:LYS:HD3  | 1.88                     | 0.53              |
| 35:1a:987:G:H2'   | 35:1a:988:G:C8     | 2.43                     | 0.53              |
| 35:1a:1323:G:H2'  | 35:1a:1324:A:H8    | 1.74                     | 0.53              |
| 35:1a:1429:A:H2'  | 35:1a:1430:A:H8    | 1.73                     | 0.53              |
| 45:1k:30:ILE:HD11 | 45:1k:43:TRP:HB2   | 1.88                     | 0.53              |
| 2:1B:95:U:H2'     | 2:1B:96:G:H8       | 1.74                     | 0.53              |
| 5:1F:103:GLY:HA2  | 5:1F:106:LYS:HD3   | 1.91                     | 0.53              |
| 15:1Q:46:ILE:O    | 15:1Q:50:ARG:HB2   | 2.07                     | 0.53              |
| 24:1Z:76:ASP:HB3  | 24:1Z:90:ASP:HB2   | 1.91                     | 0.53              |
| 40:1f:9:MET:HE1   | 40:1f:86:ARG:HH11  | 1.73                     | 0.53              |
| 1:1A:804:A:H2'    | 1:1A:806:C:C4      | 2.43                     | 0.53              |
| 7:1H:104:LEU:HB2  | 7:1H:112:VAL:HB    | 1.89                     | 0.53              |
| 20:1V:32:THR:OG1  | 20:1V:61:ALA:O     | 2.21                     | 0.53              |
| 20:1V:76:LYS:HB2  | 20:1V:85:LYS:HB3   | 1.89                     | 0.53              |
| 23:1Y:17:ASP:HB3  | 23:1Y:20:LYS:HD2   | 1.89                     | 0.53              |
| 1:1A:1264:A:H5'   | 30:15:7:PRO:HG2    | 1.91                     | 0.53              |
| 1:1A:1363:C:H2'   | 1:1A:1364:G:H8     | 1.74                     | 0.53              |
| 1:1A:2271:G:H5'   | 25:10:16:ARG:HD3   | 1.90                     | 0.53              |
| 3:1D:36:ASN:HD22  | 3:1D:61:TYR:HB2    | 1.73                     | 0.53              |
| 3:1D:169:ALA:O    | 3:1D:185:ALA:N     | 2.41                     | 0.53              |
| 18:1T:38:ARG:NH2  | 35:1a:345:C:OP2    | 2.41                     | 0.53              |
| 20:1V:98:ILE:HG22 | 20:1V:100:GLY:H    | 1.73                     | 0.53              |
| 35:1a:501:C:H2'   | 35:1a:502:A:C8     | 2.44                     | 0.53              |
| 35:1a:664:G:H22   | 35:1a:741:G:H1     | 1.56                     | 0.53              |
| 38:1d:149:LYS:NZ  | 38:1d:176:LYS:O    | 2.41                     | 0.53              |
| 1:1A:568:U:H4'    | 1:1A:945:A:N6      | 2.23                     | 0.53              |
| 1:1A:2335:A:HO2'  | 1:1A:2336:A:H8     | 1.57                     | 0.53              |
| 14:1P:56:PRO:HD2  | 14:1P:59:ARG:HD3   | 1.90                     | 0.53              |
| 15:1Q:40:ARG:HB2  | 15:1Q:93:VAL:HB    | 1.90                     | 0.53              |
| 15:1Q:105:MET:SD  | 15:1Q:108:VAL:HG21 | 2.48                     | 0.53              |
| 16:1R:103:ARG:HB2 | 16:1R:110:MET:HE3  | 1.91                     | 0.53              |
| 35:1a:35:G:O2'    | 46:1l:114:SER:O    | 2.18                     | 0.53              |
| 1:1A:248:G:O2'    | 1:1A:2432:A:OP1    | 2.17                     | 0.53              |
| 1:1A:1450:G:H21   | 1:1A:1452:G:H1     | 1.56                     | 0.53              |
| 1:1A:1844:C:H2'   | 1:1A:1845:G:C8     | 2.44                     | 0.53              |
| 35:1a:940:C:H2'   | 35:1a:941:G:C8     | 2.43                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:1a:1187:G:H4'  | 43:1i:112:ARG:NH1 | 2.24                     | 0.53              |
| 58:1x:69:G:H2'    | 58:1x:70:C:C6     | 2.42                     | 0.53              |
| 1:1A:598:U:H2'    | 1:1A:599:A:C8     | 2.44                     | 0.53              |
| 1:1A:1490:A:H62   | 3:1D:96:LYS:HB3   | 1.74                     | 0.53              |
| 35:1a:1391:U:H2'  | 35:1a:1392:G:H8   | 1.72                     | 0.53              |
| 35:1a:1437:A:H2'  | 35:1a:1438:G:H8   | 1.74                     | 0.53              |
| 37:1c:6:PRO:HD2   | 37:1c:183:TYR:CD2 | 2.44                     | 0.53              |
| 34:19:11:CYS:SG   | 34:19:33:HIS:ND1  | 2.70                     | 0.53              |
| 34:19:36:ARG:HG2  | 34:19:37:GLN:H    | 1.74                     | 0.53              |
| 35:1a:626:G:O2'   | 50:1p:51:ARG:NH1  | 2.41                     | 0.53              |
| 41:1g:72:VAL:HG12 | 41:1g:89:GLU:HG3  | 1.89                     | 0.53              |
| 1:1A:1530:G:H22   | 1:1A:1542:U:H1'   | 1.73                     | 0.53              |
| 1:1A:1814:G:H4'   | 3:1D:50:THR:HG21  | 1.90                     | 0.53              |
| 35:1a:1222:G:H5'' | 53:1s:77:ARG:HH11 | 1.73                     | 0.53              |
| 35:1a:1260:G:OP1  | 35:1a:1284:C:O2'  | 2.18                     | 0.53              |
| 46:1l:49:ARG:HB3  | 46:1l:65:TYR:HE1  | 1.74                     | 0.53              |
| 1:1A:744:U:H5''   | 1:1A:1658:C:H5''  | 1.91                     | 0.53              |
| 1:1A:1055:G:H1    | 1:1A:1104:C:H42   | 1.56                     | 0.53              |
| 1:1A:2002:G:OP2   | 16:1R:9:GLN:NE2   | 2.42                     | 0.53              |
| 1:1A:2276:G:OP2   | 15:1Q:85:GLY:N    | 2.42                     | 0.53              |
| 3:1D:69:ASN:HA    | 3:1D:188:ARG:HH12 | 1.73                     | 0.53              |
| 15:1Q:12:MET:O    | 15:1Q:86:LYS:NZ   | 2.42                     | 0.53              |
| 1:1A:968:C:H2'    | 1:1A:969:G:H8     | 1.74                     | 0.52              |
| 1:1A:1028:A:H61   | 1:1A:1125:G:H2'   | 1.74                     | 0.52              |
| 1:1A:1320:C:HO2'  | 1:1A:1321:A:H8    | 1.56                     | 0.52              |
| 1:1A:1365:A:OP1   | 26:1l:2:ARG:NH1   | 2.35                     | 0.52              |
| 1:1A:2022:U:O4    | 30:15:5:ASN:ND2   | 2.42                     | 0.52              |
| 27:12:49:ASP:OD1  | 27:12:52:ARG:NH2  | 2.42                     | 0.52              |
| 35:1a:1198:G:H2'  | 35:1a:1199:U:C6   | 2.44                     | 0.52              |
| 46:1l:32:VAL:N    | 46:1l:55:ARG:O    | 2.36                     | 0.52              |
| 1:1A:4:U:H2'      | 1:1A:5:A:C8       | 2.45                     | 0.52              |
| 1:1A:835:C:H2'    | 1:1A:836:G:H8     | 1.74                     | 0.52              |
| 1:1A:1068:G:N2    | 1:1A:1095:A:O2'   | 2.41                     | 0.52              |
| 1:1A:1129:A:O2'   | 1:1A:2515:C:O2    | 2.25                     | 0.52              |
| 1:1A:1316:U:H2'   | 1:1A:1317:G:H8    | 1.74                     | 0.52              |
| 1:1A:1916:A:H2'   | 1:1A:1917:PSU:O4' | 2.10                     | 0.52              |
| 1:1A:2189:U:H2'   | 1:1A:2190:G:H8    | 1.75                     | 0.52              |
| 9:1l:47:PHE:HA    | 9:1l:51:ARG:HB2   | 1.91                     | 0.52              |
| 33:18:13:PHE:HB3  | 33:18:21:PHE:HB3  | 1.90                     | 0.52              |
| 35:1a:877:G:H2'   | 35:1a:878:A:H8    | 1.73                     | 0.52              |
| 46:1l:28:GLN:OE1  | 46:1l:80:LEU:HD21 | 2.09                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:1q:22:VAL:O    | 51:1q:43:LEU:N     | 2.43                     | 0.52              |
| 53:1s:27:LYS:HG2  | 53:1s:28:LYS:HG2   | 1.90                     | 0.52              |
| 55:1u:13:VAL:HG13 | 55:1u:15:LEU:HG    | 1.92                     | 0.52              |
| 58:1x:74:C:N4     | 58:1x:75:C:H41     | 2.07                     | 0.52              |
| 1:1A:1320:C:N4    | 1:1A:1330:C:OP2    | 2.41                     | 0.52              |
| 1:1A:1501:G:P     | 3:1D:100:ARG:HH22  | 2.32                     | 0.52              |
| 6:1G:59:ILE:O     | 6:1G:101:ARG:NH1   | 2.42                     | 0.52              |
| 35:1a:1530:G:H2'  | 35:1a:1531:A:C8    | 2.45                     | 0.52              |
| 37:1c:83:VAL:HG13 | 37:1c:100:ILE:HD11 | 1.92                     | 0.52              |
| 47:1m:7:ASN:HB2   | 47:1m:21:ILE:HG12  | 1.92                     | 0.52              |
| 1:1A:1187:G:N2    | 1:1A:1188:U:O4     | 2.42                     | 0.52              |
| 1:1A:1283:G:N1    | 1:1A:1286:A:OP2    | 2.41                     | 0.52              |
| 1:1A:1954:G:O2'   | 1:1A:1956:U:O4     | 2.23                     | 0.52              |
| 1:1A:2120:G:H2'   | 1:1A:2121:G:C8     | 2.45                     | 0.52              |
| 1:1A:2280:G:H2'   | 1:1A:2281:A:C8     | 2.44                     | 0.52              |
| 35:1a:692:U:O2'   | 35:1a:694:A:N7     | 2.35                     | 0.52              |
| 35:1a:1201:A:H1'  | 35:1a:1202:U:OP2   | 2.09                     | 0.52              |
| 1:1A:15:G:H4'     | 30:15:17:SER:HB3   | 1.92                     | 0.52              |
| 1:1A:754:U:O2'    | 1:1A:1618:6MZ:H2   | 2.09                     | 0.52              |
| 1:1A:1038:G:H2'   | 1:1A:1039:A:C8     | 2.45                     | 0.52              |
| 35:1a:1137:C:H5'  | 35:1a:1138:G:H5'   | 1.91                     | 0.52              |
| 35:1a:1241:G:H2'  | 35:1a:1242:G:H8    | 1.74                     | 0.52              |
| 1:1A:559:G:N3     | 19:1U:55:GLN:NE2   | 2.55                     | 0.52              |
| 1:1A:690:G:N2     | 3:1D:42:ARG:HH12   | 2.07                     | 0.52              |
| 1:1A:1796:U:H3    | 1:1A:1823:G:H1     | 1.56                     | 0.52              |
| 14:1P:79:LEU:HD12 | 14:1P:114:GLY:H    | 1.73                     | 0.52              |
| 14:1P:101:ILE:HB  | 14:1P:105:ILE:HG13 | 1.90                     | 0.52              |
| 31:16:5:ARG:HG2   | 31:16:23:THR:HB    | 1.91                     | 0.52              |
| 33:18:21:PHE:O    | 33:18:49:VAL:HG23  | 2.09                     | 0.52              |
| 35:1a:401:C:H2'   | 35:1a:402:G:C8     | 2.45                     | 0.52              |
| 35:1a:1497:G:H1'  | 35:1a:1518:MA6:H2  | 1.92                     | 0.52              |
| 36:1b:95:TRP:CZ2  | 36:1b:171:ALA:HA   | 2.45                     | 0.52              |
| 1:1A:2333:A:OP1   | 25:10:73:ARG:NH2   | 2.36                     | 0.52              |
| 33:18:5:THR:HG23  | 33:18:61:LEU:HA    | 1.91                     | 0.52              |
| 35:1a:1013:G:N2   | 35:1a:1015:G:H3'   | 2.25                     | 0.52              |
| 45:1k:19:VAL:O    | 45:1k:34:THR:N     | 2.43                     | 0.52              |
| 1:1A:970:U:H2'    | 1:1A:971:G:C8      | 2.45                     | 0.52              |
| 1:1A:1924:C:H2'   | 1:1A:1925:C:C6     | 2.44                     | 0.52              |
| 1:1A:2372:U:H2'   | 1:1A:2373:G:H8     | 1.74                     | 0.52              |
| 35:1a:235:C:H2'   | 35:1a:236:A:C8     | 2.44                     | 0.52              |
| 35:1a:363:A:H5'   | 46:1l:30:ARG:HB2   | 1.92                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:1d:7:LYS:HB2    | 38:1d:20:LEU:HB3  | 1.92                     | 0.52              |
| 1:1A:500:G:N1      | 1:1A:503:A:OP2    | 2.43                     | 0.52              |
| 1:1A:2280:G:H2'    | 1:1A:2281:A:H8    | 1.75                     | 0.52              |
| 15:1Q:19:GLY:O     | 15:1Q:38:ARG:NH1  | 2.40                     | 0.52              |
| 35:1a:932:C:OP1    | 41:1g:3:ARG:NE    | 2.42                     | 0.52              |
| 50:1p:20:VAL:HG23  | 50:1p:35:ARG:HA   | 1.91                     | 0.52              |
| 54:1t:43:LYS:HD2   | 54:1t:86:ALA:HA   | 1.90                     | 0.52              |
| 1:1A:573:U:O2'     | 1:1A:575:A:OP1    | 2.22                     | 0.52              |
| 1:1A:597:G:O2'     | 14:1P:11:GLY:O    | 2.26                     | 0.52              |
| 1:1A:720:U:H2'     | 1:1A:721:A:C8     | 2.44                     | 0.52              |
| 1:1A:2101:A:H2'    | 1:1A:2102:G:C8    | 2.45                     | 0.52              |
| 28:13:53:MET:HG3   | 28:13:54:VAL:HG13 | 1.93                     | 0.52              |
| 35:1a:264:C:H4'    | 51:1q:64:ARG:HD2  | 1.92                     | 0.52              |
| 35:1a:950:U:H2'    | 35:1a:951:G:C8    | 2.43                     | 0.52              |
| 38:1d:125:ASN:HD21 | 38:1d:140:ASP:CG  | 2.18                     | 0.52              |
| 40:1f:48:ALA:N     | 52:1r:65:SER:OG   | 2.43                     | 0.52              |
| 1:1A:918:A:N3      | 2:1B:80:U:O2'     | 2.37                     | 0.51              |
| 1:1A:973:A:H5'     | 1:1A:1188:U:H1'   | 1.91                     | 0.51              |
| 1:1A:1693:U:H3'    | 1:1A:1694:C:H6    | 1.75                     | 0.51              |
| 1:1A:1919:A:O2'    | 35:1a:1517:G:N3   | 2.28                     | 0.51              |
| 4:1E:16:THR:OG1    | 4:1E:20:VAL:O     | 2.22                     | 0.51              |
| 6:1G:37:MET:HE3    | 6:1G:151:LEU:HB3  | 1.91                     | 0.51              |
| 20:1V:68:ARG:HB2   | 20:1V:90:ARG:HH21 | 1.76                     | 0.51              |
| 35:1a:545:C:OP2    | 38:1d:58:GLN:NE2  | 2.42                     | 0.51              |
| 35:1a:770:C:H2'    | 35:1a:771:G:H8    | 1.75                     | 0.51              |
| 58:1x:5:U:H3       | 58:1x:68:G:H22    | 1.57                     | 0.51              |
| 1:1A:1827:U:H5     | 3:1D:220:ARG:HD3  | 1.75                     | 0.51              |
| 1:1A:2364:C:H2'    | 1:1A:2365:G:O4'   | 2.10                     | 0.51              |
| 6:1G:63:LYS:H      | 29:14:6:HIS:CE1   | 2.29                     | 0.51              |
| 35:1a:1524:C:H2'   | 35:1a:1525:G:C8   | 2.45                     | 0.51              |
| 1:1A:415:A:O2'     | 1:1A:1866:A:OP1   | 2.29                     | 0.51              |
| 1:1A:767:U:H2'     | 1:1A:768:G:H8     | 1.76                     | 0.51              |
| 1:1A:1291:C:H2'    | 1:1A:1292:G:H8    | 1.75                     | 0.51              |
| 1:1A:1808:A:H3'    | 1:1A:1809:A:H8    | 1.76                     | 0.51              |
| 16:1R:76:VAL:HA    | 16:1R:79:LEU:HD12 | 1.91                     | 0.51              |
| 21:1W:62:ASP:OD1   | 21:1W:62:ASP:N    | 2.42                     | 0.51              |
| 23:1Y:10:VAL:HA    | 23:1Y:71:ILE:HA   | 1.91                     | 0.51              |
| 25:10:55:LEU:HD12  | 25:10:76:ILE:HD12 | 1.93                     | 0.51              |
| 36:1b:41:ASN:HD21  | 36:1b:43:GLU:HB2  | 1.75                     | 0.51              |
| 1:1A:290:U:H2'     | 1:1A:291:G:C8     | 2.45                     | 0.51              |
| 1:1A:1675:C:O2     | 4:1E:133:THR:OG1  | 2.28                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2508:G:H2'   | 1:1A:2509:G:C8    | 2.46                     | 0.51              |
| 1:1A:2757:A:OP1   | 34:19:20:ASP:N    | 2.42                     | 0.51              |
| 1:1A:2857:G:N2    | 1:1A:2860:A:OP2   | 2.35                     | 0.51              |
| 35:1a:1485:U:H2'  | 35:1a:1486:G:C8   | 2.45                     | 0.51              |
| 1:1A:414:C:O3'    | 1:1A:1878:G:N2    | 2.44                     | 0.51              |
| 1:1A:445:C:N4     | 1:1A:446:G:O6     | 2.44                     | 0.51              |
| 1:1A:883:G:N2     | 1:1A:893:C:O2     | 2.29                     | 0.51              |
| 1:1A:1509:A:H2'   | 1:1A:1510:G:C8    | 2.45                     | 0.51              |
| 1:1A:1858:A:N6    | 1:1A:1884:G:O2'   | 2.43                     | 0.51              |
| 9:1I:80:ILE:HG22  | 9:1I:82:SER:H     | 1.74                     | 0.51              |
| 35:1a:292:G:O6    | 35:1a:308:C:N4    | 2.39                     | 0.51              |
| 35:1a:303:A:O2'   | 35:1a:555:U:H4'   | 2.10                     | 0.51              |
| 35:1a:890:G:N2    | 35:1a:907:A:OP2   | 2.43                     | 0.51              |
| 35:1a:1126:U:O2'  | 35:1a:1281:C:O4'  | 2.29                     | 0.51              |
| 35:1a:1347:G:H5'' | 43:1i:108:ARG:HB2 | 1.93                     | 0.51              |
| 45:1k:30:ILE:HD13 | 45:1k:45:THR:HG22 | 1.92                     | 0.51              |
| 50:1p:8:ARG:NH1   | 50:1p:9:HIS:O     | 2.43                     | 0.51              |
| 1:1A:518:G:OP2    | 30:15:12:ARG:NH2  | 2.34                     | 0.51              |
| 1:1A:538:A:H5''   | 12:1N:7:LYS:HE3   | 1.93                     | 0.51              |
| 18:1T:47:ILE:O    | 18:1T:96:LEU:N    | 2.44                     | 0.51              |
| 19:1U:17:LEU:HA   | 19:1U:20:ALA:HB3  | 1.92                     | 0.51              |
| 35:1a:419:C:OP1   | 35:1a:513:C:O2'   | 2.27                     | 0.51              |
| 35:1a:709:U:H2'   | 35:1a:710:G:C8    | 2.45                     | 0.51              |
| 44:1j:22:THR:HG21 | 44:1j:39:PRO:HB3  | 1.93                     | 0.51              |
| 45:1k:92:ARG:NH2  | 45:1k:111:ASP:OD1 | 2.43                     | 0.51              |
| 55:1u:36:PHE:HA   | 55:1u:39:LYS:HD3  | 1.93                     | 0.51              |
| 1:1A:910:A:N3     | 1:1A:2264:C:O2'   | 2.36                     | 0.51              |
| 15:1Q:33:LEU:HD23 | 15:1Q:103:TYR:HD2 | 1.76                     | 0.51              |
| 15:1Q:53:MET:HE2  | 15:1Q:63:ILE:HG21 | 1.93                     | 0.51              |
| 47:1m:85:TYR:N    | 53:1s:72:GLU:O    | 2.44                     | 0.51              |
| 48:1n:61:ARG:HH21 | 48:1n:70:PRO:HB2  | 1.75                     | 0.51              |
| 58:1x:71:C:H2'    | 58:1x:72:U:C6     | 2.45                     | 0.51              |
| 1:1A:2361:G:O3'   | 33:18:27:ASN:ND2  | 2.44                     | 0.51              |
| 13:1O:29:HIS:ND1  | 13:1O:29:HIS:O    | 2.43                     | 0.51              |
| 35:1a:882:C:N4    | 46:1l:5:GLN:OE1   | 2.44                     | 0.51              |
| 54:1t:70:LYS:HG3  | 54:1t:73:ARG:NH2  | 2.25                     | 0.51              |
| 1:1A:1566:A:O2'   | 1:1A:1568:G:N2    | 2.44                     | 0.51              |
| 1:1A:2020:A:H61   | 1:1A:2034:U:H3    | 1.57                     | 0.51              |
| 1:1A:2440:C:H5''  | 1:1A:2587:A:H4'   | 1.93                     | 0.51              |
| 35:1a:563:A:O2'   | 35:1a:566:G:O3'   | 2.29                     | 0.51              |
| 36:1b:165:ALA:HB3 | 36:1b:190:SER:HB3 | 1.93                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:1p:46:LYS:NZ    | 50:1p:48:GLU:HB3   | 2.26                     | 0.51              |
| 1:1A:233:A:H61     | 1:1A:428:A:H61     | 1.59                     | 0.51              |
| 1:1A:514:A:N3      | 1:1A:581:C:O2'     | 2.44                     | 0.51              |
| 1:1A:1225:G:H5'    | 20:1V:88:GLY:H     | 1.75                     | 0.51              |
| 4:1E:4:LEU:HD23    | 4:1E:32:ASN:HD22   | 1.76                     | 0.51              |
| 35:1a:1108:G:H5'   | 37:1c:175:HIS:ND1  | 2.26                     | 0.51              |
| 52:1r:32:ILE:HG22  | 52:1r:38:ILE:HA    | 1.92                     | 0.51              |
| 1:1A:24:G:H2'      | 1:1A:25:U:C6       | 2.46                     | 0.50              |
| 1:1A:951:C:H2'     | 1:1A:952:G:H8      | 1.76                     | 0.50              |
| 1:1A:1019:U:H3     | 1:1A:1142:A:H62    | 1.57                     | 0.50              |
| 1:1A:1432:G:H2'    | 1:1A:1433:A:C8     | 2.46                     | 0.50              |
| 1:1A:2039:U:H2'    | 1:1A:2040:G:H8     | 1.76                     | 0.50              |
| 1:1A:2238:G:N2     | 1:1A:2238:G:OP2    | 2.44                     | 0.50              |
| 35:1a:537:G:H5''   | 46:1l:109:ARG:HH12 | 1.75                     | 0.50              |
| 35:1a:545:C:H5''   | 38:1d:68:GLU:HG2   | 1.93                     | 0.50              |
| 35:1a:726:C:H2'    | 35:1a:727:G:C8     | 2.46                     | 0.50              |
| 35:1a:835:U:OP1    | 52:1r:52:ARG:NH2   | 2.39                     | 0.50              |
| 35:1a:1464:U:H2'   | 35:1a:1465:A:C8    | 2.46                     | 0.50              |
| 37:1c:105:VAL:HG22 | 37:1c:107:LYS:H    | 1.76                     | 0.50              |
| 1:1A:414:C:H2'     | 1:1A:415:A:C8      | 2.47                     | 0.50              |
| 1:1A:1028:A:N3     | 1:1A:2486:C:O2'    | 2.39                     | 0.50              |
| 2:1B:24:G:N2       | 2:1B:27:C:N3       | 2.58                     | 0.50              |
| 3:1D:77:VAL:HA     | 3:1D:93:VAL:HA     | 1.94                     | 0.50              |
| 22:1X:13:ALA:H     | 22:1X:33:LYS:HB2   | 1.77                     | 0.50              |
| 35:1a:240:G:H2'    | 35:1a:241:G:H8     | 1.77                     | 0.50              |
| 35:1a:776:G:N2     | 35:1a:802:A:OP2    | 2.42                     | 0.50              |
| 35:1a:1306:A:N6    | 35:1a:1331:G:O2'   | 2.44                     | 0.50              |
| 36:1b:56:LEU:HD13  | 36:1b:216:VAL:HG13 | 1.92                     | 0.50              |
| 50:1p:23:ASP:HB3   | 50:1p:26:ASN:HD22  | 1.76                     | 0.50              |
| 1:1A:13:A:O2'      | 1:1A:15:G:N7       | 2.39                     | 0.50              |
| 1:1A:1567:G:H3'    | 3:1D:84:PRO:HG3    | 1.92                     | 0.50              |
| 1:1A:2820:A:H4'    | 16:1R:3:HIS:CD2    | 2.46                     | 0.50              |
| 2:1B:45:A:O4'      | 6:1G:91:ARG:NH2    | 2.44                     | 0.50              |
| 10:1J:59:LEU:HB3   | 10:1J:62:ARG:HB3   | 1.92                     | 0.50              |
| 35:1a:1134:G:H1    | 35:1a:1140:C:H42   | 1.60                     | 0.50              |
| 39:1e:10:LEU:HD22  | 39:1e:67:ARG:HH22  | 1.76                     | 0.50              |
| 47:1m:82:LEU:HB3   | 53:1s:73:PHE:HE1   | 1.76                     | 0.50              |
| 49:1o:44:GLU:O     | 49:1o:46:LYS:N     | 2.45                     | 0.50              |
| 1:1A:505:A:O2'     | 1:1A:509:C:O2'     | 2.29                     | 0.50              |
| 1:1A:619:G:H3'     | 1:1A:620:G:H21     | 1.77                     | 0.50              |
| 36:1b:12:GLY:HA3   | 36:1b:207:ARG:HD3  | 1.93                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 55:1u:36:PHE:O     | 55:1u:38:GLU:N    | 2.44                     | 0.50              |
| 1:1A:328:U:H4'     | 23:1Y:65:GLN:HG3  | 1.94                     | 0.50              |
| 1:1A:775:G:H4'     | 1:1A:776:G:O5'    | 2.10                     | 0.50              |
| 1:1A:2258:C:O2'    | 1:1A:2427:C:OP2   | 2.25                     | 0.50              |
| 1:1A:2443:C:H2'    | 1:1A:2444:G:H8    | 1.77                     | 0.50              |
| 3:1D:51:ARG:HH22   | 3:1D:246:PRO:HG2  | 1.75                     | 0.50              |
| 3:1D:129:LEU:HD13  | 3:1D:133:ASN:HB2  | 1.92                     | 0.50              |
| 37:1c:55:VAL:HB    | 37:1c:66:THR:HB   | 1.92                     | 0.50              |
| 1:1A:819:A:H3'     | 1:1A:973:A:H61    | 1.75                     | 0.50              |
| 4:1E:25:THR:HG21   | 4:1E:193:VAL:HG21 | 1.94                     | 0.50              |
| 6:1G:116:LEU:HD13  | 6:1G:175:PRO:HG2  | 1.94                     | 0.50              |
| 13:1O:16:ALA:HA    | 13:1O:46:ALA:HA   | 1.94                     | 0.50              |
| 14:1P:79:LEU:H     | 14:1P:113:ALA:HB3 | 1.77                     | 0.50              |
| 35:1a:684:U:H1'    | 45:1k:39:ASN:HB2  | 1.92                     | 0.50              |
| 43:1i:68:GLY:O     | 43:1i:74:GLN:NE2  | 2.40                     | 0.50              |
| 1:1A:516:C:OP1     | 30:15:9:ARG:NH1   | 2.44                     | 0.50              |
| 1:1A:803:U:O4      | 1:1A:804:A:N6     | 2.45                     | 0.50              |
| 1:1A:2221:G:H2'    | 1:1A:2222:C:C6    | 2.46                     | 0.50              |
| 1:1A:2472:G:H2'    | 1:1A:2475:C:H42   | 1.77                     | 0.50              |
| 5:1F:97:ASN:HB2    | 5:1F:100:MET:HG3  | 1.93                     | 0.50              |
| 47:1m:113:LYS:H    | 47:1m:114:PRO:HD2 | 1.77                     | 0.50              |
| 1:1A:119:A:H4'     | 1:1A:120:U:H5'    | 1.93                     | 0.50              |
| 35:1a:257:G:H2'    | 35:1a:258:G:C8    | 2.45                     | 0.50              |
| 35:1a:407:U:H2'    | 35:1a:408:A:C8    | 2.46                     | 0.50              |
| 35:1a:500:G:N2     | 35:1a:546:A:H1'   | 2.27                     | 0.50              |
| 40:1f:51:ILE:HG21  | 40:1f:86:ARG:HH12 | 1.77                     | 0.50              |
| 1:1A:1:G:H1        | 1:1A:2902:C:H42   | 1.58                     | 0.50              |
| 1:1A:1059:G:H5'    | 1:1A:1060:U:OP2   | 2.12                     | 0.50              |
| 1:1A:1597:A:H5''   | 1:1A:1598:A:H5'   | 1.93                     | 0.50              |
| 1:1A:1949:G:H1     | 1:1A:1957:C:H42   | 1.60                     | 0.50              |
| 3:1D:70:LYS:HB3    | 3:1D:73:ILE:HD12  | 1.94                     | 0.50              |
| 35:1a:952:U:H2'    | 35:1a:953:G:C8    | 2.46                     | 0.50              |
| 36:1b:110:ILE:HG23 | 36:1b:151:LYS:HA  | 1.94                     | 0.50              |
| 46:1l:66:ILE:HG21  | 46:1l:71:HIS:CD2  | 2.47                     | 0.50              |
| 58:1x:41:G:H2'     | 58:1x:42:U:C6     | 2.47                     | 0.50              |
| 1:1A:729:G:H5''    | 1:1A:730:A:H5''   | 1.94                     | 0.49              |
| 1:1A:1190:G:H2'    | 1:1A:1191:G:C8    | 2.47                     | 0.49              |
| 1:1A:2002:G:H5''   | 16:1R:9:GLN:HE21  | 1.77                     | 0.49              |
| 1:1A:2270:A:H2'    | 1:1A:2271:G:O4'   | 2.12                     | 0.49              |
| 2:1B:114:C:H2'     | 2:1B:115:A:C8     | 2.47                     | 0.49              |
| 10:1J:3:LEU:HD12   | 10:1J:5:LEU:H     | 1.76                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:1c:146:LYS:HB2 | 37:1c:202:PHE:HD2  | 1.76                     | 0.49              |
| 1:1A:2696:U:H2'   | 1:1A:2697:G:H8     | 1.77                     | 0.49              |
| 1:1A:2808:G:O2'   | 1:1A:2809:A:H8     | 1.94                     | 0.49              |
| 4:1E:51:THR:HB    | 4:1E:79:LEU:HD23   | 1.94                     | 0.49              |
| 5:1F:47:LYS:HB2   | 5:1F:51:GLU:HB2    | 1.94                     | 0.49              |
| 35:1a:579:A:H2'   | 35:1a:580:C:C6     | 2.47                     | 0.49              |
| 1:1A:1415:U:H3    | 1:1A:1587:G:H1     | 1.60                     | 0.49              |
| 1:1A:1818:U:H4'   | 1:1A:1821:A:H1'    | 1.93                     | 0.49              |
| 1:1A:2345:G:H4'   | 1:1A:2346:A:H3'    | 1.93                     | 0.49              |
| 2:1B:105:G:H2'    | 2:1B:106:G:H8      | 1.77                     | 0.49              |
| 2:1B:118:C:H2'    | 2:1B:119:A:H8      | 1.78                     | 0.49              |
| 3:1D:143:VAL:HB   | 3:1D:153:LEU:HB2   | 1.94                     | 0.49              |
| 5:1F:49:ARG:HD2   | 5:1F:76:PRO:HD3    | 1.94                     | 0.49              |
| 9:1I:63:ALA:HB1   | 9:1I:135:HIS:HE2   | 1.77                     | 0.49              |
| 13:1O:19:VAL:HA   | 13:1O:44:LYS:H     | 1.77                     | 0.49              |
| 38:1d:57:LYS:HD3  | 38:1d:202:LEU:HD22 | 1.93                     | 0.49              |
| 40:1f:32:ALA:HB1  | 40:1f:67:PRO:HD2   | 1.94                     | 0.49              |
| 49:1o:35:ILE:HG22 | 49:1o:39:GLN:HE21  | 1.78                     | 0.49              |
| 1:1A:18:U:OP1     | 19:1U:25:GLY:N     | 2.44                     | 0.49              |
| 1:1A:249:C:O2     | 33:18:11:LYS:NZ    | 2.45                     | 0.49              |
| 1:1A:655:A:H4'    | 1:1A:656:G:H5'     | 1.92                     | 0.49              |
| 1:1A:946:C:H2'    | 1:1A:947:A:H8      | 1.77                     | 0.49              |
| 1:1A:1899:A:H4'   | 1:1A:1901:A:H5''   | 1.94                     | 0.49              |
| 1:1A:2566:A:H4'   | 1:1A:2567:G:O5'    | 2.11                     | 0.49              |
| 25:10:61:GLY:HA3  | 25:10:79:GLU:O     | 2.13                     | 0.49              |
| 1:1A:1528:A:OP2   | 1:1A:1543:G:N2     | 2.46                     | 0.49              |
| 1:1A:2059:A:N6    | 1:1A:2503:2MA:H2'  | 2.27                     | 0.49              |
| 1:1A:2284:A:H1'   | 1:1A:2325:G:N1     | 2.27                     | 0.49              |
| 3:1D:2:VAL:HG13   | 3:1D:18:VAL:HG22   | 1.95                     | 0.49              |
| 3:1D:72:GLY:N     | 3:1D:117:SER:O     | 2.35                     | 0.49              |
| 21:1W:80:PRO:O    | 21:1W:100:THR:OG1  | 2.28                     | 0.49              |
| 35:1a:1017:U:H2'  | 35:1a:1018:G:H8    | 1.78                     | 0.49              |
| 1:1A:191:A:H2'    | 1:1A:192:C:C6      | 2.47                     | 0.49              |
| 1:1A:341:C:H2'    | 1:1A:342:A:C8      | 2.48                     | 0.49              |
| 1:1A:839:U:H3     | 1:1A:939:G:H1      | 1.59                     | 0.49              |
| 1:1A:939:G:H2'    | 1:1A:940:G:C8      | 2.48                     | 0.49              |
| 1:1A:1693:U:O2'   | 3:1D:13:ARG:NH1    | 2.45                     | 0.49              |
| 1:1A:1752:C:H2'   | 1:1A:1753:G:C8     | 2.48                     | 0.49              |
| 1:1A:1871:A:H8    | 1:1A:1872:A:C8     | 2.30                     | 0.49              |
| 1:1A:2496:C:N3    | 1:1A:2498:OMC:N4   | 2.60                     | 0.49              |
| 16:1R:24:MET:HE3  | 16:1R:44:LEU:HD13  | 1.93                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:10:19:VAL:HG13 | 25:10:34:VAL:HG22  | 1.94                     | 0.49              |
| 36:1b:80:LYS:HB2  | 36:1b:92:ASN:HD22  | 1.78                     | 0.49              |
| 1:1A:2257:U:O4    | 1:1A:2258:C:N4     | 2.46                     | 0.49              |
| 2:1B:48:U:H5'     | 17:1S:98:GLN:HB3   | 1.94                     | 0.49              |
| 11:1K:63:ASP:O    | 11:1K:65:SER:N     | 2.46                     | 0.49              |
| 35:1a:717:U:H5''  | 35:1a:734:G:OP2    | 2.12                     | 0.49              |
| 35:1a:979:C:H1'   | 35:1a:1317:C:H41   | 1.78                     | 0.49              |
| 35:1a:1486:G:H2'  | 35:1a:1487:G:C8    | 2.47                     | 0.49              |
| 1:1A:151:C:H2'    | 1:1A:152:A:H8      | 1.78                     | 0.49              |
| 1:1A:373:U:H1'    | 1:1A:423:A:N3      | 2.27                     | 0.49              |
| 1:1A:860:U:H2'    | 1:1A:861:A:H8      | 1.76                     | 0.49              |
| 1:1A:907:G:N2     | 15:1Q:70:ASP:OD2   | 2.46                     | 0.49              |
| 1:1A:1320:C:O2'   | 1:1A:1321:A:H8     | 1.96                     | 0.49              |
| 1:1A:2331:G:H4'   | 25:10:39:THR:H     | 1.78                     | 0.49              |
| 1:1A:2417:C:H2'   | 1:1A:2418:A:C8     | 2.48                     | 0.49              |
| 1:1A:2651:C:H2'   | 1:1A:2652:C:C6     | 2.48                     | 0.49              |
| 3:1D:65:ASP:HB2   | 3:1D:101:ARG:HB3   | 1.95                     | 0.49              |
| 35:1a:284:C:H2'   | 35:1a:285:C:C6     | 2.48                     | 0.49              |
| 35:1a:662:U:H2'   | 35:1a:663:A:C8     | 2.48                     | 0.49              |
| 35:1a:1464:U:H2'  | 35:1a:1465:A:H8    | 1.76                     | 0.49              |
| 42:1h:94:VAL:HB   | 42:1h:99:GLY:O     | 2.13                     | 0.49              |
| 45:1k:46:ALA:HA   | 45:1k:65:ALA:HB2   | 1.95                     | 0.49              |
| 52:1r:25:ILE:HA   | 52:1r:28:LEU:HB3   | 1.94                     | 0.49              |
| 1:1A:185:G:H2'    | 1:1A:186:G:H8      | 1.78                     | 0.49              |
| 1:1A:768:G:N2     | 1:1A:1379:U:O2'    | 2.45                     | 0.49              |
| 1:1A:784:G:C6     | 3:1D:227:VAL:HG11  | 2.47                     | 0.49              |
| 1:1A:832:U:H2'    | 1:1A:833:A:C8      | 2.47                     | 0.49              |
| 1:1A:2245:U:H5''  | 1:1A:2246:G:H5'    | 1.94                     | 0.49              |
| 2:1B:76:G:P       | 24:1Z:9:ARG:HH22   | 2.35                     | 0.49              |
| 6:1G:56:LEU:O     | 6:1G:60:SER:OG     | 2.19                     | 0.49              |
| 7:1H:68:ARG:HH12  | 7:1H:72:ASN:ND2    | 2.10                     | 0.49              |
| 20:1V:68:ARG:HH11 | 20:1V:90:ARG:HB2   | 1.78                     | 0.49              |
| 35:1a:707:U:H2'   | 35:1a:708:C:C6     | 2.48                     | 0.49              |
| 37:1c:122:GLN:HG2 | 37:1c:125:ARG:HH22 | 1.77                     | 0.49              |
| 42:1h:65:PHE:CD2  | 42:1h:66:GLN:HG2   | 2.47                     | 0.49              |
| 1:1A:606:U:H4'    | 1:1A:658:U:O2'     | 2.13                     | 0.49              |
| 1:1A:1930:G:N1    | 1:1A:1968:G:N7     | 2.61                     | 0.49              |
| 1:1A:2082:A:H2'   | 1:1A:2083:G:O4'    | 2.12                     | 0.49              |
| 1:1A:2141:G:H2'   | 1:1A:2142:A:H8     | 1.77                     | 0.49              |
| 1:1A:2326:C:O2'   | 1:1A:2327:A:OP1    | 2.29                     | 0.49              |
| 1:1A:2489:U:O2'   | 1:1A:2518:A:N6     | 2.46                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2845:U:H2'   | 1:1A:2846:G:C8    | 2.47                     | 0.49              |
| 11:1K:107:GLU:O   | 11:1K:110:GLN:NE2 | 2.44                     | 0.49              |
| 35:1a:85:U:H4'    | 35:1a:86:G:O5'    | 2.12                     | 0.49              |
| 35:1a:1003:G:N2   | 35:1a:1037:C:O2   | 2.36                     | 0.49              |
| 39:1e:59:ILE:O    | 39:1e:63:MET:HG2  | 2.12                     | 0.49              |
| 1:1A:693:A:O2'    | 1:1A:1353:A:N3    | 2.45                     | 0.48              |
| 1:1A:721:A:H2'    | 1:1A:722:A:C8     | 2.47                     | 0.48              |
| 1:1A:1181:U:H2'   | 1:1A:1182:G:H8    | 1.78                     | 0.48              |
| 1:1A:1407:G:H2'   | 1:1A:1408:G:H8    | 1.78                     | 0.48              |
| 1:1A:2011:U:H2'   | 1:1A:2012:G:O4'   | 2.12                     | 0.48              |
| 5:1F:48:THR:OG1   | 5:1F:51:GLU:OE1   | 2.22                     | 0.48              |
| 15:1Q:12:MET:HG2  | 15:1Q:72:PRO:HG2  | 1.95                     | 0.48              |
| 35:1a:654:G:O6    | 35:1a:754:C:N4    | 2.38                     | 0.48              |
| 35:1a:782:A:H62   | 35:1a:800:G:H21   | 1.60                     | 0.48              |
| 35:1a:940:C:H2'   | 35:1a:941:G:H8    | 1.78                     | 0.48              |
| 41:1g:74:VAL:HG12 | 41:1g:87:PRO:HB3  | 1.95                     | 0.48              |
| 48:1n:37:SER:HA   | 48:1n:41:ARG:HB2  | 1.93                     | 0.48              |
| 58:1x:71:C:H2'    | 58:1x:72:U:H6     | 1.78                     | 0.48              |
| 1:1A:534:U:H2'    | 1:1A:535:G:H8     | 1.77                     | 0.48              |
| 1:1A:977:G:H2'    | 1:1A:978:G:H8     | 1.78                     | 0.48              |
| 1:1A:1266:G:N2    | 1:1A:1267:U:O4    | 2.30                     | 0.48              |
| 1:1A:1415:U:H2'   | 1:1A:1416:G:H4'   | 1.95                     | 0.48              |
| 1:1A:1682:G:C4    | 1:1A:1757:A:H1'   | 2.47                     | 0.48              |
| 1:1A:1794:A:H2'   | 1:1A:1795:C:C6    | 2.47                     | 0.48              |
| 1:1A:2039:U:H2'   | 1:1A:2040:G:C8    | 2.48                     | 0.48              |
| 1:1A:2233:U:H2'   | 1:1A:2234:G:H8    | 1.78                     | 0.48              |
| 1:1A:2258:C:C4    | 1:1A:2426:A:H5'   | 2.47                     | 0.48              |
| 1:1A:2431:U:O2'   | 1:1A:2433:A:N7    | 2.40                     | 0.48              |
| 1:1A:2794:C:H42   | 1:1A:2802:G:H1    | 1.59                     | 0.48              |
| 5:1F:143:LEU:HB3  | 5:1F:146:VAL:HG11 | 1.95                     | 0.48              |
| 17:1S:39:VAL:N    | 17:1S:49:VAL:O    | 2.38                     | 0.48              |
| 23:1Y:3:LYS:HB3   | 23:1Y:82:VAL:HG21 | 1.96                     | 0.48              |
| 28:13:8:GLN:HB2   | 28:13:28:LEU:HD13 | 1.95                     | 0.48              |
| 35:1a:1200:C:O2'  | 35:1a:1205:U:O4   | 2.31                     | 0.48              |
| 35:1a:1308:U:H2'  | 35:1a:1309:G:C8   | 2.47                     | 0.48              |
| 41:1g:56:SER:OG   | 41:1g:57:GLU:OE1  | 2.27                     | 0.48              |
| 43:1i:62:LEU:HB3  | 43:1i:64:ILE:HG13 | 1.94                     | 0.48              |
| 1:1A:599:A:H2'    | 1:1A:600:G:C8     | 2.48                     | 0.48              |
| 1:1A:765:C:H2'    | 1:1A:766:U:H6     | 1.77                     | 0.48              |
| 1:1A:877:A:O2'    | 1:1A:900:A:N6     | 2.47                     | 0.48              |
| 1:1A:2120:G:H2'   | 1:1A:2121:G:H8    | 1.77                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:2418:A:P      | 33:18:44:ARG:HH21 | 2.36                     | 0.48              |
| 2:1B:88:C:O2'      | 2:1B:89:U:O5'     | 2.23                     | 0.48              |
| 4:1E:24:VAL:HG12   | 4:1E:178:VAL:HG21 | 1.94                     | 0.48              |
| 6:1G:12:VAL:O      | 6:1G:16:MET:HG2   | 2.14                     | 0.48              |
| 11:1K:20:SER:HB3   | 11:1K:21:PRO:HD3  | 1.95                     | 0.48              |
| 35:1a:811:C:O2'    | 35:1a:901:A:N1    | 2.47                     | 0.48              |
| 35:1a:837:U:H2'    | 35:1a:838:G:C8    | 2.49                     | 0.48              |
| 35:1a:1230:C:H2'   | 35:1a:1231:G:H8   | 1.78                     | 0.48              |
| 1:1A:581:C:H2'     | 1:1A:582:A:H8     | 1.76                     | 0.48              |
| 1:1A:663:G:H5''    | 14:1P:17:LYS:HD3  | 1.94                     | 0.48              |
| 1:1A:966:G:H2'     | 1:1A:967:U:C6     | 2.48                     | 0.48              |
| 2:1B:28:C:H2'      | 2:1B:29:A:H8      | 1.78                     | 0.48              |
| 3:1D:140:VAL:HG12  | 3:1D:191:LEU:HD23 | 1.94                     | 0.48              |
| 11:1K:91:LYS:HG3   | 11:1K:94:LYS:HE2  | 1.95                     | 0.48              |
| 14:1P:71:ALA:O     | 14:1P:74:THR:HG22 | 2.14                     | 0.48              |
| 14:1P:73:ILE:HD12  | 14:1P:106:GLU:HB2 | 1.95                     | 0.48              |
| 35:1a:1429:A:H2'   | 35:1a:1430:A:C8   | 2.48                     | 0.48              |
| 44:1j:8:ILE:HB     | 44:1j:74:VAL:HB   | 1.96                     | 0.48              |
| 45:1k:51:PHE:HA    | 45:1k:55:ARG:HE   | 1.78                     | 0.48              |
| 1:1A:1355:G:H2'    | 1:1A:1356:G:H8    | 1.79                     | 0.48              |
| 1:1A:2374:C:N4     | 1:1A:2375:G:O6    | 2.46                     | 0.48              |
| 11:1K:33:ASN:OD1   | 11:1K:34:ILE:N    | 2.46                     | 0.48              |
| 20:1V:79:ARG:C     | 20:1V:81:LYS:H    | 2.21                     | 0.48              |
| 28:13:23:LEU:HD21  | 28:13:53:MET:SD   | 2.53                     | 0.48              |
| 33:18:25:HIS:CE1   | 33:18:47:ALA:HB2  | 2.48                     | 0.48              |
| 35:1a:754:C:O2     | 35:1a:754:C:H2'   | 2.12                     | 0.48              |
| 35:1a:1250:A:H2'   | 35:1a:1251:A:C8   | 2.48                     | 0.48              |
| 45:1k:21:HIS:O     | 45:1k:32:THR:N    | 2.31                     | 0.48              |
| 56:1v:26:G:C6      | 57:1w:442:TRP:HH2 | 2.31                     | 0.48              |
| 1:1A:630:G:N2      | 1:1A:633:A:OP2    | 2.38                     | 0.48              |
| 1:1A:633:A:O2'     | 1:1A:2404:U:OP1   | 2.29                     | 0.48              |
| 1:1A:1775:U:H2'    | 1:1A:1776:G:O4'   | 2.12                     | 0.48              |
| 1:1A:1836:C:H2'    | 1:1A:1837:C:H6    | 1.79                     | 0.48              |
| 1:1A:2313:C:H2'    | 1:1A:2314:A:C8    | 2.48                     | 0.48              |
| 7:1H:21:GLN:NE2    | 7:1H:40:VAL:O     | 2.34                     | 0.48              |
| 32:17:30:VAL:O     | 32:17:34:ARG:HG2  | 2.13                     | 0.48              |
| 35:1a:35:G:O2'     | 46:1l:117:GLY:HA2 | 2.13                     | 0.48              |
| 35:1a:194:C:H5'    | 54:1t:55:PRO:HA   | 1.96                     | 0.48              |
| 35:1a:1165:U:H2'   | 35:1a:1166:G:C8   | 2.47                     | 0.48              |
| 35:1a:1351:U:H3    | 35:1a:1371:G:H1   | 1.62                     | 0.48              |
| 36:1b:162:VAL:HG12 | 36:1b:164:ASP:H   | 1.79                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:1c:149:LYS:HG3  | 37:1c:168:ARG:HB3  | 1.96                     | 0.48              |
| 39:1e:106:ALA:HB1  | 39:1e:110:MET:HE3  | 1.95                     | 0.48              |
| 43:1i:33:SER:HB3   | 43:1i:36:GLN:HG2   | 1.95                     | 0.48              |
| 1:1A:2623:G:H2'    | 1:1A:2624:G:C8     | 2.49                     | 0.48              |
| 1:1A:2724:U:H2'    | 1:1A:2725:A:C8     | 2.49                     | 0.48              |
| 6:1G:9:ASP:OD1     | 6:1G:9:ASP:N       | 2.46                     | 0.48              |
| 35:1a:118:U:H3'    | 35:1a:288:A:H61    | 1.78                     | 0.48              |
| 45:1k:62:ALA:HB1   | 45:1k:95:THR:HB    | 1.96                     | 0.48              |
| 1:1A:729:G:N2      | 3:1D:10:PRO:O      | 2.47                     | 0.48              |
| 1:1A:813:U:H2'     | 1:1A:814:C:C6      | 2.49                     | 0.48              |
| 1:1A:1777:U:H3     | 1:1A:1787:A:H61    | 1.60                     | 0.48              |
| 3:1D:106:PRO:HD2   | 3:1D:109:LEU:HD22  | 1.95                     | 0.48              |
| 14:1P:57:LEU:HD22  | 33:18:53:ASP:HB3   | 1.95                     | 0.48              |
| 17:1S:40:ILE:HG12  | 17:1S:47:VAL:HG12  | 1.96                     | 0.48              |
| 19:1U:68:ALA:HB1   | 19:1U:73:ILE:HG23  | 1.94                     | 0.48              |
| 19:1U:111:LYS:HB2  | 20:1V:48:LYS:HD2   | 1.95                     | 0.48              |
| 35:1a:1287:A:C2    | 35:1a:1353:G:H1'   | 2.48                     | 0.48              |
| 35:1a:1497:G:C2'   | 35:1a:1498:UR3:H5' | 2.44                     | 0.48              |
| 37:1c:137:VAL:HG21 | 37:1c:167:TYR:HD2  | 1.79                     | 0.48              |
| 38:1d:97:LEU:HB2   | 38:1d:134:TYR:HB3  | 1.95                     | 0.48              |
| 43:1i:39:GLY:HA2   | 43:1i:44:ARG:HB2   | 1.96                     | 0.48              |
| 47:1m:9:PRO:HB2    | 47:1m:12:LYS:HD2   | 1.96                     | 0.48              |
| 50:1p:46:LYS:HG3   | 50:1p:48:GLU:H     | 1.79                     | 0.48              |
| 51:1q:22:VAL:N     | 51:1q:43:LEU:O     | 2.45                     | 0.48              |
| 1:1A:85:G:OP1      | 23:1Y:6:ARG:N      | 2.46                     | 0.48              |
| 1:1A:672:C:H2'     | 1:1A:673:C:C6      | 2.49                     | 0.48              |
| 1:1A:696:G:N2      | 1:1A:767:U:H1'     | 2.29                     | 0.48              |
| 1:1A:832:U:H5'     | 14:1P:38:GLN:HB3   | 1.96                     | 0.48              |
| 1:1A:1278:C:H2'    | 1:1A:1279:G:H8     | 1.79                     | 0.48              |
| 1:1A:2051:A:H2'    | 1:1A:2578:G:OP1    | 2.13                     | 0.48              |
| 1:1A:2286:G:H4'    | 1:1A:2287:A:O5'    | 2.13                     | 0.48              |
| 10:1J:59:LEU:HG    | 10:1J:61:ARG:H     | 1.79                     | 0.48              |
| 14:1P:30:THR:HG21  | 14:1P:35:HIS:CD2   | 2.49                     | 0.48              |
| 35:1a:484:G:H4'    | 35:1a:485:U:H5''   | 1.94                     | 0.48              |
| 35:1a:993:G:O2'    | 35:1a:994:A:N7     | 2.47                     | 0.48              |
| 35:1a:1291:U:H2'   | 35:1a:1292:G:H8    | 1.79                     | 0.48              |
| 35:1a:1417:G:H2'   | 35:1a:1482:G:N2    | 2.29                     | 0.48              |
| 1:1A:465:G:P       | 32:17:12:ARG:HH12  | 2.36                     | 0.48              |
| 1:1A:1636:U:H2'    | 1:1A:1637:A:C8     | 2.49                     | 0.48              |
| 1:1A:2593:U:H2'    | 1:1A:2594:C:C6     | 2.49                     | 0.48              |
| 1:1A:2696:U:H2'    | 1:1A:2697:G:C8     | 2.49                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:1I:132:PHE:HB2  | 9:1I:140:ALA:HB3  | 1.96                     | 0.48              |
| 13:1O:34:GLY:O    | 13:1O:36:GLY:N    | 2.45                     | 0.48              |
| 35:1a:253:A:H2'   | 35:1a:254:G:C8    | 2.49                     | 0.48              |
| 35:1a:298:A:H2'   | 35:1a:299:G:O4'   | 2.14                     | 0.48              |
| 35:1a:500:G:H22   | 35:1a:546:A:H1'   | 1.79                     | 0.48              |
| 35:1a:979:C:H1'   | 35:1a:1317:C:N4   | 2.28                     | 0.48              |
| 35:1a:1106:G:O2'  | 37:1c:168:ARG:NH1 | 2.47                     | 0.48              |
| 35:1a:1302:C:H42  | 47:1m:13:HIS:CD2  | 2.31                     | 0.48              |
| 38:1d:149:LYS:NZ  | 38:1d:177:MET:HB2 | 2.28                     | 0.48              |
| 50:1p:46:LYS:HZ2  | 50:1p:48:GLU:HB3  | 1.78                     | 0.48              |
| 7:1H:41:GLU:HB2   | 7:1H:54:ARG:HB2   | 1.95                     | 0.47              |
| 19:1U:87:VAL:HG12 | 19:1U:89:ILE:H    | 1.79                     | 0.47              |
| 35:1a:1296:C:N4   | 35:1a:1297:G:O6   | 2.47                     | 0.47              |
| 35:1a:1320:C:H2'  | 35:1a:1321:U:C6   | 2.49                     | 0.47              |
| 35:1a:1329:A:H5'' | 47:1m:24:VAL:HA   | 1.96                     | 0.47              |
| 1:1A:151:C:H2'    | 1:1A:152:A:C8     | 2.49                     | 0.47              |
| 1:1A:2052:A:H2'   | 1:1A:2053:G:H8    | 1.78                     | 0.47              |
| 1:1A:2233:U:H2'   | 1:1A:2234:G:C8    | 2.49                     | 0.47              |
| 1:1A:2297:A:N6    | 1:1A:2319:G:H1'   | 2.29                     | 0.47              |
| 1:1A:2680:U:O2'   | 4:1E:11:MET:SD    | 2.72                     | 0.47              |
| 10:1J:67:THR:HG21 | 10:1J:75:ALA:HB2  | 1.96                     | 0.47              |
| 23:1Y:73:ASN:HA   | 23:1Y:95:PHE:CE1  | 2.49                     | 0.47              |
| 42:1h:86:LYS:HB2  | 42:1h:91:LEU:HD23 | 1.96                     | 0.47              |
| 1:1A:1836:C:H2'   | 1:1A:1837:C:C6    | 2.49                     | 0.47              |
| 1:1A:1993:U:H4'   | 4:1E:133:THR:HG21 | 1.95                     | 0.47              |
| 1:1A:2453:A:H2'   | 1:1A:2454:G:H8    | 1.79                     | 0.47              |
| 1:1A:2470:G:O6    | 1:1A:2476:A:O2'   | 2.23                     | 0.47              |
| 2:1B:3:C:H3'      | 2:1B:4:C:H5''     | 1.96                     | 0.47              |
| 2:1B:80:U:H2'     | 2:1B:81:G:H8      | 1.79                     | 0.47              |
| 9:1I:51:ARG:HA    | 9:1I:55:GLU:HB2   | 1.97                     | 0.47              |
| 23:1Y:80:ASP:OD2  | 23:1Y:95:PHE:HB3  | 2.14                     | 0.47              |
| 32:17:3:ARG:HG3   | 32:17:5:PHE:H     | 1.80                     | 0.47              |
| 35:1a:427:U:O2'   | 35:1a:541:G:OP1   | 2.32                     | 0.47              |
| 35:1a:1370:G:H2'  | 35:1a:1371:G:H8   | 1.78                     | 0.47              |
| 39:1e:82:HIS:NE2  | 39:1e:146:MET:HG3 | 2.29                     | 0.47              |
| 1:1A:1071:G:H1'   | 1:1A:1089:A:N7    | 2.29                     | 0.47              |
| 1:1A:1141:U:H4'   | 1:1A:1142:A:O4'   | 2.14                     | 0.47              |
| 13:1O:12:ASP:HB3  | 13:1O:99:ILE:HG12 | 1.96                     | 0.47              |
| 20:1V:14:VAL:HG21 | 20:1V:98:ILE:HG13 | 1.95                     | 0.47              |
| 24:1Z:76:ASP:OD1  | 24:1Z:77:VAL:N    | 2.48                     | 0.47              |
| 27:12:25:GLN:HE21 | 27:12:50:VAL:HG21 | 1.79                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:1a:690:G:OP2    | 45:1k:28:ASN:ND2  | 2.47                     | 0.47              |
| 35:1a:1096:C:H2'   | 35:1a:1097:C:C6   | 2.49                     | 0.47              |
| 35:1a:1137:C:O2'   | 35:1a:1138:G:N2   | 2.47                     | 0.47              |
| 38:1d:58:GLN:OE1   | 38:1d:61:ARG:NH1  | 2.47                     | 0.47              |
| 40:1f:32:ALA:O     | 40:1f:34:GLY:N    | 2.44                     | 0.47              |
| 40:1f:92:THR:OG1   | 40:1f:93:LYS:N    | 2.48                     | 0.47              |
| 1:1A:331:C:H41     | 1:1A:1210:G:N2    | 2.12                     | 0.47              |
| 1:1A:558:U:H2'     | 1:1A:559:G:C8     | 2.49                     | 0.47              |
| 1:1A:724:U:H2'     | 1:1A:725:G:O4'    | 2.14                     | 0.47              |
| 1:1A:1494:A:H2     | 1:1A:1579:A:H1'   | 1.80                     | 0.47              |
| 1:1A:1792:G:O2'    | 1:1A:1830:C:OP1   | 2.29                     | 0.47              |
| 1:1A:2746:U:H5''   | 7:1H:137:LYS:HE2  | 1.95                     | 0.47              |
| 5:1F:52:VAL:HG21   | 5:1F:82:GLY:H     | 1.78                     | 0.47              |
| 25:10:42:HIS:CD2   | 25:10:73:ARG:HB2  | 2.49                     | 0.47              |
| 35:1a:11:G:N2      | 35:1a:525:C:O2'   | 2.43                     | 0.47              |
| 35:1a:982:U:P      | 48:1n:63:ARG:HH22 | 2.37                     | 0.47              |
| 36:1b:101:THR:N    | 36:1b:174:GLU:OE2 | 2.46                     | 0.47              |
| 37:1c:115:VAL:HG13 | 37:1c:136:ALA:HB1 | 1.96                     | 0.47              |
| 41:1g:143:MET:O    | 41:1g:147:ASN:HB3 | 2.14                     | 0.47              |
| 1:1A:196:A:OP2     | 14:1P:47:ARG:NH1  | 2.47                     | 0.47              |
| 1:1A:1005:C:H2'    | 1:1A:1006:C:C6    | 2.49                     | 0.47              |
| 1:1A:1562:U:H2'    | 1:1A:1563:U:C6    | 2.48                     | 0.47              |
| 1:1A:1636:U:H2'    | 1:1A:1637:A:H8    | 1.79                     | 0.47              |
| 10:1J:77:VAL:HG13  | 10:1J:114:GLU:OE2 | 2.15                     | 0.47              |
| 23:1Y:24:VAL:HA    | 23:1Y:35:VAL:HG22 | 1.96                     | 0.47              |
| 32:17:34:ARG:NH2   | 32:17:41:ARG:O    | 2.48                     | 0.47              |
| 36:1b:124:THR:HA   | 36:1b:127:LYS:HG2 | 1.96                     | 0.47              |
| 54:1t:67:HIS:ND1   | 54:1t:67:HIS:O    | 2.48                     | 0.47              |
| 1:1A:742:A:H2'     | 1:1A:743:A:H8     | 1.80                     | 0.47              |
| 1:1A:780:G:O2'     | 1:1A:783:A:N6     | 2.44                     | 0.47              |
| 1:1A:937:C:OP2     | 33:18:51:LYS:NZ   | 2.47                     | 0.47              |
| 1:1A:1187:G:H5''   | 20:1V:83:TYR:CZ   | 2.48                     | 0.47              |
| 1:1A:1751:U:H2'    | 1:1A:1752:C:C6    | 2.50                     | 0.47              |
| 1:1A:1795:C:O2'    | 1:1A:1901:A:OP2   | 2.24                     | 0.47              |
| 1:1A:1863:G:H4'    | 1:1A:2411:A:H4'   | 1.96                     | 0.47              |
| 1:1A:1916:A:N1     | 35:1a:1408:A:H4'  | 2.29                     | 0.47              |
| 1:1A:2259:U:O2     | 1:1A:2282:G:N2    | 2.45                     | 0.47              |
| 1:1A:2417:C:H2'    | 1:1A:2418:A:H8    | 1.80                     | 0.47              |
| 1:1A:2537:U:H2'    | 1:1A:2538:C:C6    | 2.49                     | 0.47              |
| 1:1A:2773:C:OP1    | 4:1E:169:ARG:NH2  | 2.48                     | 0.47              |
| 1:1A:2819:G:H2'    | 1:1A:2821:A:N7    | 2.30                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2851:A:O3'    | 16:1R:64:ARG:NH2   | 2.48                     | 0.47              |
| 3:1D:172:THR:HA    | 3:1D:182:LYS:HA    | 1.97                     | 0.47              |
| 15:1Q:22:GLN:O     | 15:1Q:24:THR:N     | 2.48                     | 0.47              |
| 15:1Q:53:MET:HE1   | 15:1Q:117:PHE:HE1  | 1.79                     | 0.47              |
| 32:17:37:LYS:NZ    | 32:17:39:ARG:HH21  | 2.13                     | 0.47              |
| 35:1a:59:A:H3'     | 35:1a:331:G:H22    | 1.80                     | 0.47              |
| 35:1a:201:G:O2'    | 35:1a:469:C:O2'    | 2.29                     | 0.47              |
| 35:1a:1017:U:H2'   | 35:1a:1018:G:C8    | 2.49                     | 0.47              |
| 35:1a:1182:G:H5'   | 35:1a:1183:U:OP1   | 2.14                     | 0.47              |
| 35:1a:1297:G:H4'   | 35:1a:1298:U:O5'   | 2.14                     | 0.47              |
| 43:1i:30:ASN:O     | 43:1i:32:ARG:N     | 2.41                     | 0.47              |
| 43:1i:91:GLU:OE2   | 43:1i:94:ARG:NH1   | 2.47                     | 0.47              |
| 1:1A:129:C:H2'     | 1:1A:130:C:C6      | 2.49                     | 0.47              |
| 1:1A:171:U:H2'     | 1:1A:172:A:H8      | 1.80                     | 0.47              |
| 1:1A:179:C:H2'     | 1:1A:180:G:C8      | 2.50                     | 0.47              |
| 1:1A:259:G:O2'     | 1:1A:621:A:O2'     | 2.26                     | 0.47              |
| 1:1A:534:U:H2'     | 1:1A:535:G:C8      | 2.50                     | 0.47              |
| 1:1A:690:G:H2'     | 1:1A:691:C:C6      | 2.50                     | 0.47              |
| 1:1A:2809:A:H2'    | 1:1A:2810:A:C8     | 2.49                     | 0.47              |
| 10:1J:18:VAL:HA    | 10:1J:86:MET:HE2   | 1.97                     | 0.47              |
| 14:1P:85:VAL:HG13  | 14:1P:98:ALA:HB2   | 1.97                     | 0.47              |
| 14:1P:110:VAL:HG21 | 14:1P:127:VAL:HG22 | 1.97                     | 0.47              |
| 18:1T:26:GLU:HA    | 18:1T:43:GLU:HA    | 1.96                     | 0.47              |
| 35:1a:107:G:OP1    | 35:1a:325:A:N6     | 2.48                     | 0.47              |
| 35:1a:126:G:OP1    | 35:1a:605:U:O2'    | 2.30                     | 0.47              |
| 35:1a:780:A:N6     | 35:1a:801:U:OP2    | 2.46                     | 0.47              |
| 42:1h:103:VAL:HA   | 42:1h:124:ILE:HA   | 1.96                     | 0.47              |
| 43:1i:101:GLY:O    | 43:1i:103:VAL:N    | 2.46                     | 0.47              |
| 1:1A:227:A:C2      | 1:1A:228:C:H1'     | 2.50                     | 0.47              |
| 1:1A:682:G:O6      | 1:1A:794:A:N6      | 2.48                     | 0.47              |
| 1:1A:2732:G:P      | 4:1E:208:LYS:HZ3   | 2.37                     | 0.47              |
| 35:1a:696:A:N3     | 35:1a:786:G:O2'    | 2.39                     | 0.47              |
| 35:1a:755:G:H21    | 42:1h:3:GLN:HE22   | 1.61                     | 0.47              |
| 42:1h:79:ARG:HH21  | 42:1h:82:LEU:HD22  | 1.80                     | 0.47              |
| 53:1s:52:ASN:HD21  | 53:1s:55:GLN:HB2   | 1.79                     | 0.47              |
| 1:1A:271:G:H1'     | 1:1A:272:A:C8      | 2.50                     | 0.47              |
| 1:1A:789:A:N6      | 32:17:3:ARG:HH12   | 2.13                     | 0.47              |
| 1:1A:1048:A:OP2    | 1:1A:1110:G:N2     | 2.48                     | 0.47              |
| 1:1A:1218:G:OP2    | 19:1U:14:LYS:NZ    | 2.41                     | 0.47              |
| 1:1A:1571:A:H2'    | 1:1A:1572:A:C8     | 2.50                     | 0.47              |
| 4:1E:121:THR:HG21  | 4:1E:143:PRO:HB3   | 1.97                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:1I:20:ASN:OD1    | 9:1I:21:VAL:N      | 2.48                     | 0.47              |
| 35:1a:19:A:OP1     | 39:1e:134:ASN:ND2  | 2.48                     | 0.47              |
| 35:1a:407:U:H2'    | 35:1a:408:A:H8     | 1.80                     | 0.47              |
| 36:1b:53:LEU:HD23  | 36:1b:56:LEU:HD12  | 1.96                     | 0.47              |
| 38:1d:77:GLU:O     | 38:1d:81:LEU:HG    | 2.15                     | 0.47              |
| 3:1D:130:PRO:HA    | 3:1D:188:ARG:HA    | 1.98                     | 0.46              |
| 9:1I:3:VAL:HA      | 9:1I:38:PRO:HA     | 1.96                     | 0.46              |
| 35:1a:19:A:H5'     | 39:1e:90:GLY:HA3   | 1.96                     | 0.46              |
| 35:1a:948:C:H5'    | 35:1a:1306:A:O2'   | 2.15                     | 0.46              |
| 37:1c:2:GLN:N      | 37:1c:2:GLN:OE1    | 2.47                     | 0.46              |
| 1:1A:1808:A:H3'    | 1:1A:1809:A:C8     | 2.51                     | 0.46              |
| 1:1A:2086:U:H2'    | 1:1A:2087:G:C8     | 2.51                     | 0.46              |
| 1:1A:2314:A:H2'    | 1:1A:2315:G:C8     | 2.50                     | 0.46              |
| 1:1A:2339:C:H2'    | 1:1A:2340:A:H8     | 1.79                     | 0.46              |
| 3:1D:259:ASN:O     | 3:1D:261:ARG:N     | 2.41                     | 0.46              |
| 3:1D:267:VAL:HG12  | 3:1D:268:ARG:HG2   | 1.96                     | 0.46              |
| 15:1Q:102:LEU:HD11 | 15:1Q:126:ILE:HD11 | 1.97                     | 0.46              |
| 30:15:51:ARG:HD2   | 30:15:53:VAL:HG12  | 1.97                     | 0.46              |
| 45:1k:12:ARG:O     | 45:1k:14:GLN:N     | 2.39                     | 0.46              |
| 1:1A:839:U:H2'     | 1:1A:840:C:C6      | 2.51                     | 0.46              |
| 1:1A:2522:U:O2'    | 1:1A:2647:U:OP1    | 2.26                     | 0.46              |
| 4:1E:29:VAL:O      | 4:1E:185:ASN:HB3   | 2.14                     | 0.46              |
| 35:1a:401:C:H2'    | 35:1a:402:G:H8     | 1.80                     | 0.46              |
| 36:1b:198:VAL:HG22 | 36:1b:200:PRO:HD3  | 1.97                     | 0.46              |
| 1:1A:528:A:C2      | 1:1A:2042:A:H2'    | 2.51                     | 0.46              |
| 1:1A:537:G:H22     | 1:1A:555:G:H2'     | 1.80                     | 0.46              |
| 1:1A:565:C:N4      | 1:1A:575:A:H61     | 2.14                     | 0.46              |
| 1:1A:1190:G:H2'    | 1:1A:1191:G:H8     | 1.80                     | 0.46              |
| 1:1A:2194:U:H2'    | 1:1A:2195:U:C6     | 2.50                     | 0.46              |
| 1:1A:2267:A:H5''   | 1:1A:2268:A:H5'    | 1.98                     | 0.46              |
| 1:1A:2357:G:P      | 25:10:16:ARG:HE    | 2.39                     | 0.46              |
| 1:1A:2601:C:H5''   | 58:1x:75:C:OP1     | 2.15                     | 0.46              |
| 15:1Q:29:GLY:HA2   | 15:1Q:106:ASP:HB2  | 1.97                     | 0.46              |
| 35:1a:287:U:H2'    | 35:1a:288:A:C8     | 2.51                     | 0.46              |
| 35:1a:375:U:OP1    | 50:1p:70:ARG:HD3   | 2.15                     | 0.46              |
| 1:1A:336:C:H2'     | 1:1A:337:C:C6      | 2.51                     | 0.46              |
| 1:1A:355:U:H2'     | 1:1A:356:G:H8      | 1.80                     | 0.46              |
| 1:1A:948:C:O2      | 1:1A:984:A:O2'     | 2.14                     | 0.46              |
| 1:1A:2146:C:H4'    | 1:1A:2147:A:C5     | 2.50                     | 0.46              |
| 6:1G:129:MET:HG2   | 6:1G:153:ILE:HB    | 1.96                     | 0.46              |
| 35:1a:734:G:O2'    | 52:1r:59:LYS:HD3   | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:1a:1317:C:H4'   | 48:1n:48:LEU:HD21  | 1.98                     | 0.46              |
| 36:1b:93:HIS:CE1   | 36:1b:145:ASN:HB2  | 2.50                     | 0.46              |
| 39:1e:35:LEU:HD22  | 39:1e:133:ILE:HG13 | 1.97                     | 0.46              |
| 48:1n:35:ASN:OD1   | 48:1n:35:ASN:N     | 2.47                     | 0.46              |
| 52:1r:45:GLY:O     | 52:1r:46:THR:OG1   | 2.29                     | 0.46              |
| 1:1A:968:C:H2'     | 1:1A:969:G:C8      | 2.51                     | 0.46              |
| 1:1A:2144:G:O2'    | 1:1A:2147:A:N1     | 2.45                     | 0.46              |
| 2:1B:38:C:H2'      | 2:1B:39:A:C8       | 2.50                     | 0.46              |
| 2:1B:71:C:H42      | 2:1B:105:G:H1      | 1.64                     | 0.46              |
| 21:1W:20:VAL:HG11  | 21:1W:44:ALA:HA    | 1.98                     | 0.46              |
| 35:1a:1067:A:N1    | 35:1a:1108:G:O2'   | 2.49                     | 0.46              |
| 35:1a:1238:A:OP1   | 35:1a:1335:U:O2'   | 2.21                     | 0.46              |
| 41:1g:128:GLU:OE1  | 41:1g:128:GLU:N    | 2.48                     | 0.46              |
| 1:1A:233:A:N6      | 1:1A:428:A:H61     | 2.13                     | 0.46              |
| 1:1A:438:G:H2'     | 1:1A:439:A:C8      | 2.51                     | 0.46              |
| 1:1A:1146:C:H2'    | 1:1A:1147:A:C8     | 2.50                     | 0.46              |
| 1:1A:1238:G:H2'    | 1:1A:1239:G:H8     | 1.80                     | 0.46              |
| 1:1A:1667:G:N2     | 1:1A:1992:G:OP2    | 2.47                     | 0.46              |
| 1:1A:1843:C:H42    | 1:1A:1897:G:H1     | 1.63                     | 0.46              |
| 3:1D:137:GLY:HA2   | 3:1D:163:ILE:O     | 2.15                     | 0.46              |
| 15:1Q:47:GLU:OE2   | 15:1Q:51:ARG:NE    | 2.47                     | 0.46              |
| 35:1a:106:C:O2'    | 35:1a:379:C:OP1    | 2.33                     | 0.46              |
| 35:1a:458:U:H2'    | 35:1a:459:A:C8     | 2.51                     | 0.46              |
| 35:1a:496:A:H61    | 35:1a:498:A:H62    | 1.62                     | 0.46              |
| 35:1a:708:C:H2'    | 35:1a:709:U:C6     | 2.50                     | 0.46              |
| 35:1a:1437:A:H2'   | 35:1a:1438:G:C8    | 2.50                     | 0.46              |
| 37:1c:148:ILE:HG13 | 37:1c:201:ILE:HG12 | 1.98                     | 0.46              |
| 1:1A:18:U:H2'      | 1:1A:19:A:C8       | 2.51                     | 0.46              |
| 1:1A:440:C:H2'     | 1:1A:441:U:C6      | 2.51                     | 0.46              |
| 1:1A:807:U:H4'     | 1:1A:2446:G:OP1    | 2.16                     | 0.46              |
| 1:1A:863:A:H2'     | 1:1A:864:G:C8      | 2.50                     | 0.46              |
| 1:1A:942:G:H2'     | 1:1A:943:A:O4'     | 2.15                     | 0.46              |
| 1:1A:1345:C:H2'    | 1:1A:1346:G:H8     | 1.81                     | 0.46              |
| 1:1A:1397:U:N3     | 1:1A:1602:U:O2     | 2.49                     | 0.46              |
| 1:1A:1672:A:C2     | 1:1A:2582:G:H5'    | 2.51                     | 0.46              |
| 1:1A:2519:U:H5'    | 1:1A:2567:G:H21    | 1.80                     | 0.46              |
| 15:1Q:110:GLU:OE2  | 15:1Q:114:ARG:NH1  | 2.49                     | 0.46              |
| 35:1a:556:C:H2'    | 35:1a:557:G:H8     | 1.80                     | 0.46              |
| 35:1a:1002:G:N2    | 35:1a:1038:C:O2    | 2.29                     | 0.46              |
| 35:1a:1222:G:H5''  | 53:1s:77:ARG:HD3   | 1.97                     | 0.46              |
| 35:1a:1289:A:C8    | 35:1a:1290:G:C8    | 3.04                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:1g:129:ASN:O   | 41:1g:134:VAL:HG21 | 2.16                     | 0.46              |
| 46:1l:85:ARG:HA   | 46:1l:93:ARG:HA    | 1.98                     | 0.46              |
| 1:1A:160:A:H2'    | 1:1A:161:A:C8      | 2.50                     | 0.46              |
| 1:1A:334:C:OP1    | 1:1A:335:C:N4      | 2.48                     | 0.46              |
| 1:1A:357:C:H2'    | 1:1A:358:U:C6      | 2.51                     | 0.46              |
| 1:1A:2572:A:OP2   | 4:1E:149:ASN:HB3   | 2.16                     | 0.46              |
| 1:1A:2845:U:O3'   | 18:1T:52:ARG:NH1   | 2.49                     | 0.46              |
| 6:1G:97:GLU:HG2   | 29:14:25:ARG:HB2   | 1.98                     | 0.46              |
| 11:1K:4:VAL:HA    | 11:1K:7:TYR:CE2    | 2.51                     | 0.46              |
| 13:1O:109:SER:O   | 13:1O:111:LYS:N    | 2.49                     | 0.46              |
| 16:1R:29:VAL:HG13 | 16:1R:83:LEU:HD11  | 1.98                     | 0.46              |
| 35:1a:86:G:H4'    | 35:1a:87:C:O5'     | 2.16                     | 0.46              |
| 35:1a:837:U:H2'   | 35:1a:838:G:H8     | 1.81                     | 0.46              |
| 35:1a:952:U:H5'   | 35:1a:972:C:N4     | 2.31                     | 0.46              |
| 35:1a:1289:A:H3'  | 35:1a:1290:G:H8    | 1.80                     | 0.46              |
| 38:1d:74:TYR:OH   | 38:1d:96:ARG:NH1   | 2.49                     | 0.46              |
| 39:1e:15:ILE:HD12 | 39:1e:36:THR:HA    | 1.98                     | 0.46              |
| 44:1j:80:THR:HG22 | 44:1j:82:LYS:H     | 1.81                     | 0.46              |
| 1:1A:976:G:O2'    | 1:1A:1155:A:O2'    | 2.20                     | 0.46              |
| 1:1A:2828:G:H2'   | 1:1A:2829:A:H8     | 1.80                     | 0.46              |
| 2:1B:13:G:N2      | 2:1B:16:G:O2'      | 2.49                     | 0.46              |
| 22:1X:37:ASP:O    | 22:1X:81:LYS:NZ    | 2.45                     | 0.46              |
| 33:18:38:LYS:HG3  | 33:18:41:ARG:HH11  | 1.81                     | 0.46              |
| 35:1a:755:G:H2'   | 35:1a:756:C:C6     | 2.51                     | 0.46              |
| 35:1a:778:G:O2'   | 45:1k:120:CYS:HB2  | 2.16                     | 0.46              |
| 35:1a:1233:G:O2'  | 35:1a:1365:G:OP1   | 2.26                     | 0.46              |
| 38:1d:28:ASP:OD1  | 38:1d:28:ASP:N     | 2.47                     | 0.46              |
| 38:1d:71:PHE:HA   | 38:1d:74:TYR:HD2   | 1.80                     | 0.46              |
| 40:1f:26:THR:HA   | 40:1f:29:ILE:HD12  | 1.98                     | 0.46              |
| 43:1i:122:ARG:NH1 | 43:1i:123:ARG:O    | 2.49                     | 0.46              |
| 50:1p:76:LYS:O    | 50:1p:79:ASN:ND2   | 2.49                     | 0.46              |
| 58:1x:11:C:H2'    | 58:1x:12:U:C6      | 2.50                     | 0.46              |
| 1:1A:281:C:N3     | 1:1A:359:G:N2      | 2.63                     | 0.45              |
| 1:1A:1935:G:N2    | 1:1A:1964:G:O4'    | 2.45                     | 0.45              |
| 1:1A:2557:G:H2'   | 1:1A:2558:C:C6     | 2.51                     | 0.45              |
| 1:1A:2818:U:H2'   | 1:1A:2819:G:C8     | 2.51                     | 0.45              |
| 4:1E:151:THR:HB   | 4:1E:152:PRO:HD3   | 1.98                     | 0.45              |
| 9:1I:30:LEU:HA    | 9:1I:35:LYS:HB2    | 1.98                     | 0.45              |
| 35:1a:405:U:O4    | 38:1d:1:ALA:N      | 2.37                     | 0.45              |
| 35:1a:504:C:H2'   | 35:1a:511:C:C5     | 2.50                     | 0.45              |
| 35:1a:676:A:H1'   | 45:1k:116:PRO:HB3  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:1a:876:C:H2'   | 35:1a:877:G:C8    | 2.51                     | 0.45              |
| 35:1a:948:C:H2'   | 35:1a:949:A:H8    | 1.81                     | 0.45              |
| 35:1a:1038:C:H2'  | 35:1a:1039:G:C8   | 2.50                     | 0.45              |
| 35:1a:1236:A:H4'  | 35:1a:1304:G:H4'  | 1.98                     | 0.45              |
| 36:1b:100:LEU:HB2 | 36:1b:174:GLU:HG2 | 1.97                     | 0.45              |
| 1:1A:326:G:H2'    | 1:1A:327:G:C8     | 2.51                     | 0.45              |
| 1:1A:341:C:H2'    | 1:1A:342:A:H8     | 1.81                     | 0.45              |
| 1:1A:625:G:H2'    | 1:1A:626:A:C8     | 2.50                     | 0.45              |
| 1:1A:805:G:N2     | 1:1A:829:A:OP1    | 2.50                     | 0.45              |
| 1:1A:2060:A:H3'   | 5:1F:63:LYS:NZ    | 2.31                     | 0.45              |
| 1:1A:2336:A:N3    | 1:1A:2385:C:H1'   | 2.31                     | 0.45              |
| 1:1A:2884:U:H2'   | 1:1A:2885:G:H8    | 1.82                     | 0.45              |
| 12:1N:36:LEU:HD22 | 12:1N:121:LYS:HB2 | 1.98                     | 0.45              |
| 30:15:30:ASP:HB3  | 30:15:34:GLY:H    | 1.81                     | 0.45              |
| 35:1a:272:C:H2'   | 35:1a:273:U:C6    | 2.51                     | 0.45              |
| 35:1a:437:U:O2'   | 38:1d:119:HIS:ND1 | 2.38                     | 0.45              |
| 35:1a:693:G:H2'   | 35:1a:694:A:O4'   | 2.16                     | 0.45              |
| 35:1a:801:U:H2'   | 35:1a:802:A:H8    | 1.80                     | 0.45              |
| 35:1a:1143:G:H2'  | 35:1a:1144:G:C8   | 2.51                     | 0.45              |
| 43:1i:11:ARG:H    | 43:1i:77:ALA:HA   | 1.81                     | 0.45              |
| 46:1l:32:VAL:HB   | 46:1l:55:ARG:HB3  | 1.99                     | 0.45              |
| 1:1A:1:G:H2'      | 1:1A:2:G:H8       | 1.82                     | 0.45              |
| 1:1A:560:C:O2'    | 19:1U:47:ARG:NH2  | 2.49                     | 0.45              |
| 3:1D:51:ARG:HH12  | 3:1D:246:PRO:HG2  | 1.82                     | 0.45              |
| 6:1G:104:THR:HA   | 29:14:38:SER:HB3  | 1.98                     | 0.45              |
| 11:1K:57:VAL:HG23 | 11:1K:71:LYS:HZ2  | 1.81                     | 0.45              |
| 15:1Q:53:MET:HE2  | 15:1Q:63:ILE:HD13 | 1.98                     | 0.45              |
| 35:1a:254:G:N2    | 51:1q:17:GLU:OE1  | 2.29                     | 0.45              |
| 35:1a:911:U:OP2   | 46:1l:93:ARG:NH1  | 2.49                     | 0.45              |
| 35:1a:1432:G:N2   | 35:1a:1468:A:OP2  | 2.49                     | 0.45              |
| 44:1j:42:LEU:HD11 | 44:1j:73:LEU:HG   | 1.98                     | 0.45              |
| 55:1u:32:ARG:HG3  | 55:1u:33:ARG:H    | 1.81                     | 0.45              |
| 1:1A:395:U:H2'    | 1:1A:396:G:C8     | 2.52                     | 0.45              |
| 1:1A:876:C:H2'    | 1:1A:877:A:O4'    | 2.16                     | 0.45              |
| 1:1A:972:A:OP2    | 1:1A:973:A:O2'    | 2.27                     | 0.45              |
| 1:1A:1485:U:H2'   | 1:1A:1486:U:C6    | 2.50                     | 0.45              |
| 1:1A:2400:G:H1    | 1:1A:2416:C:H42   | 1.64                     | 0.45              |
| 1:1A:2615:U:C2    | 30:15:3:GLN:HA    | 2.51                     | 0.45              |
| 1:1A:2651:C:H2'   | 1:1A:2652:C:H6    | 1.82                     | 0.45              |
| 5:1F:189:THR:HG22 | 5:1F:191:ASP:H    | 1.80                     | 0.45              |
| 45:1k:108:ASN:HB3 | 55:1u:6:ARG:HG3   | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:1p:61:VAL:HG22  | 50:1p:67:ILE:HD11  | 1.98                     | 0.45              |
| 1:1A:46:G:H2'      | 1:1A:47:C:C6       | 2.51                     | 0.45              |
| 1:1A:286:U:H2'     | 1:1A:287:G:C8      | 2.51                     | 0.45              |
| 1:1A:355:U:H2'     | 1:1A:356:G:C8      | 2.51                     | 0.45              |
| 1:1A:372:G:O2'     | 1:1A:373:U:O5'     | 2.31                     | 0.45              |
| 1:1A:764:A:H5'     | 3:1D:208:GLY:HA3   | 1.99                     | 0.45              |
| 1:1A:801:G:C8      | 5:1F:50:ALA:HB2    | 2.51                     | 0.45              |
| 1:1A:2251:OMG:HM22 | 1:1A:2251:OMG:H1'  | 1.62                     | 0.45              |
| 12:1N:95:ARG:HG2   | 12:1N:96:ARG:HG2   | 1.97                     | 0.45              |
| 14:1P:127:VAL:HG21 | 14:1P:142:ILE:HG21 | 1.98                     | 0.45              |
| 35:1a:1174:G:H2'   | 35:1a:1175:G:H8    | 1.82                     | 0.45              |
| 46:1l:73:LEU:HD21  | 46:1l:79:ILE:HG21  | 1.99                     | 0.45              |
| 54:1t:28:ARG:HA    | 54:1t:31:ILE:HD12  | 1.98                     | 0.45              |
| 1:1A:126:A:N6      | 32:17:42:LEU:HD23  | 2.32                     | 0.45              |
| 1:1A:519:U:H2'     | 1:1A:520:G:H8      | 1.81                     | 0.45              |
| 1:1A:1026:G:H2'    | 1:1A:1027:A:H8     | 1.81                     | 0.45              |
| 1:1A:1326:U:H2'    | 1:1A:1327:A:C8     | 2.52                     | 0.45              |
| 1:1A:1363:C:H2'    | 1:1A:1364:G:C8     | 2.50                     | 0.45              |
| 1:1A:2377:A:H2'    | 1:1A:2378:A:C8     | 2.52                     | 0.45              |
| 1:1A:2622:U:O2'    | 1:1A:2825:G:N7     | 2.50                     | 0.45              |
| 2:1B:52:A:N6       | 17:1S:33:ARG:HB2   | 2.31                     | 0.45              |
| 3:1D:203:VAL:O     | 3:1D:205:GLY:N     | 2.49                     | 0.45              |
| 9:1I:113:SER:O     | 9:1I:116:ARG:NH1   | 2.36                     | 0.45              |
| 10:1J:24:SER:HB2   | 10:1J:116:GLU:HG3  | 1.99                     | 0.45              |
| 32:17:24:THR:HG23  | 32:17:27:GLY:H     | 1.82                     | 0.45              |
| 35:1a:132:C:H5''   | 54:1t:67:HIS:HE1   | 1.80                     | 0.45              |
| 35:1a:599:C:H2'    | 35:1a:600:A:C8     | 2.52                     | 0.45              |
| 35:1a:1326:U:H2'   | 35:1a:1327:C:C6    | 2.52                     | 0.45              |
| 45:1k:49:SER:OG    | 45:1k:68:ARG:HD3   | 2.17                     | 0.45              |
| 53:1s:36:ARG:H     | 53:1s:36:ARG:HG2   | 1.58                     | 0.45              |
| 56:1v:23:U:H2'     | 56:1v:24:C:C6      | 2.52                     | 0.45              |
| 1:1A:819:A:H5'     | 1:1A:973:A:N1      | 2.31                     | 0.45              |
| 1:1A:1288:G:OP2    | 1:1A:1288:G:N2     | 2.30                     | 0.45              |
| 1:1A:2646:C:H2'    | 1:1A:2647:U:O4'    | 2.16                     | 0.45              |
| 4:1E:16:THR:OG1    | 4:1E:18:ASP:OD1    | 2.35                     | 0.45              |
| 9:1I:108:VAL:HG12  | 9:1I:110:VAL:H     | 1.82                     | 0.45              |
| 11:1K:112:LYS:HE2  | 11:1K:128:ILE:HD13 | 1.99                     | 0.45              |
| 13:1O:48:PRO:HG3   | 35:1a:1422:G:OP1   | 2.17                     | 0.45              |
| 15:1Q:30:SER:N     | 15:1Q:105:MET:O    | 2.50                     | 0.45              |
| 35:1a:376:G:H2'    | 35:1a:377:G:C8     | 2.52                     | 0.45              |
| 35:1a:439:U:H2'    | 35:1a:440:C:O4'    | 2.17                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:1a:1291:U:H2'    | 35:1a:1292:G:C8    | 2.52                     | 0.45              |
| 35:1a:1343:G:H4'    | 43:1i:123:ARG:HB2  | 1.99                     | 0.45              |
| 35:1a:1478:U:H2'    | 35:1a:1479:C:C6    | 2.52                     | 0.45              |
| 1:1A:1103:A:H3'     | 1:1A:1104:C:H5''   | 1.98                     | 0.45              |
| 1:1A:1825:U:H1'     | 3:1D:252:LYS:HE3   | 1.98                     | 0.45              |
| 1:1A:1882:U:H2'     | 1:1A:1883:U:C6     | 2.51                     | 0.45              |
| 1:1A:2742:G:OP2     | 34:19:24:ARG:NH1   | 2.50                     | 0.45              |
| 4:1E:13:ARG:HH11    | 18:1T:55:HIS:HA    | 1.82                     | 0.45              |
| 29:14:57:VAL:HG22   | 53:1s:66:VAL:HG21  | 1.97                     | 0.45              |
| 32:17:12:ARG:HE     | 32:17:44:VAL:HG21  | 1.81                     | 0.45              |
| 35:1a:601:G:H2'     | 35:1a:602:A:C8     | 2.52                     | 0.45              |
| 35:1a:674:G:N2      | 35:1a:717:U:O2     | 2.48                     | 0.45              |
| 38:1d:191:SER:OG    | 38:1d:194:ILE:HG12 | 2.17                     | 0.45              |
| 41:1g:56:SER:HB3    | 41:1g:59:GLU:HG2   | 1.99                     | 0.45              |
| 1:1A:18:U:O2'       | 1:1A:554:U:OP1     | 2.35                     | 0.45              |
| 1:1A:460:A:H62      | 1:1A:469:G:H21     | 1.64                     | 0.45              |
| 1:1A:774:G:O2'      | 1:1A:777:G:N3      | 2.46                     | 0.45              |
| 1:1A:1345:C:H2'     | 1:1A:1346:G:C8     | 2.52                     | 0.45              |
| 1:1A:2236:U:H2'     | 1:1A:2237:G:O4'    | 2.17                     | 0.45              |
| 3:1D:52:HIS:HA      | 3:1D:216:ARG:HB3   | 1.98                     | 0.45              |
| 5:1F:18:THR:HG23    | 5:1F:106:LYS:HG2   | 1.98                     | 0.45              |
| 15:1Q:40:ARG:HB3    | 15:1Q:95:LEU:HD23  | 1.99                     | 0.45              |
| 35:1a:186:C:O2'     | 54:1t:75:LYS:O     | 2.29                     | 0.45              |
| 35:1a:526:C:H2'     | 35:1a:527:7MG:H4'  | 1.98                     | 0.45              |
| 35:1a:1250:A:H61    | 35:1a:1354:U:H1'   | 1.82                     | 0.45              |
| 35:1a:1402:4OC:HM22 | 35:1a:1402:4OC:H1' | 1.55                     | 0.45              |
| 37:1c:122:GLN:HG2   | 37:1c:125:ARG:HH12 | 1.82                     | 0.45              |
| 42:1h:76:ARG:HH12   | 42:1h:125:ILE:HG23 | 1.82                     | 0.45              |
| 1:1A:1251:C:H5''    | 19:1U:5:ARG:NH2    | 2.32                     | 0.45              |
| 1:1A:1434:A:H2'     | 1:1A:1435:G:C8     | 2.52                     | 0.45              |
| 1:1A:1783:A:N1      | 1:1A:2587:A:H2'    | 2.32                     | 0.45              |
| 1:1A:2590:A:H5''    | 3:1D:237:ARG:NE    | 2.32                     | 0.45              |
| 3:1D:154:ALA:HB2    | 3:1D:161:VAL:HG23  | 1.98                     | 0.45              |
| 7:1H:37:ASN:OD1     | 7:1H:38:ASP:N      | 2.50                     | 0.45              |
| 11:1K:101:SER:HA    | 11:1K:140:GLU:H    | 1.82                     | 0.45              |
| 24:1Z:2:PHE:O       | 24:1Z:62:THR:OG1   | 2.26                     | 0.45              |
| 35:1a:379:C:N4      | 35:1a:380:G:O6     | 2.50                     | 0.45              |
| 35:1a:1175:G:H2'    | 35:1a:1176:A:H8    | 1.82                     | 0.45              |
| 35:1a:1481:U:H2'    | 35:1a:1482:G:C8    | 2.51                     | 0.45              |
| 1:1A:171:U:H2'      | 1:1A:172:A:C8      | 2.52                     | 0.44              |
| 1:1A:453:A:N3       | 1:1A:457:A:O2'     | 2.46                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:1813:G:O6     | 1:1A:1814:G:N1    | 2.50                     | 0.44              |
| 3:1D:70:LYS:HD2    | 3:1D:73:ILE:HD12  | 1.98                     | 0.44              |
| 7:1H:97:VAL:HG22   | 7:1H:102:ILE:HG23 | 1.98                     | 0.44              |
| 27:12:10:SER:HA    | 27:12:13:GLU:HG2  | 1.99                     | 0.44              |
| 35:1a:146:G:N2     | 35:1a:177:G:N7    | 2.64                     | 0.44              |
| 35:1a:345:C:O2'    | 35:1a:346:G:N2    | 2.50                     | 0.44              |
| 35:1a:1391:U:H2'   | 35:1a:1392:G:C8   | 2.51                     | 0.44              |
| 37:1c:137:VAL:HG21 | 37:1c:167:TYR:CD2 | 2.51                     | 0.44              |
| 45:1k:24:ALA:N     | 45:1k:86:LYS:O    | 2.49                     | 0.44              |
| 46:1l:41:PRO:HD2   | 46:1l:47:ALA:N    | 2.29                     | 0.44              |
| 51:1q:26:ARG:HG3   | 51:1q:39:ARG:HB2  | 1.99                     | 0.44              |
| 1:1A:320:A:H4'     | 1:1A:322:A:N7     | 2.32                     | 0.44              |
| 1:1A:961:C:O2      | 1:1A:2031:A:N6    | 2.50                     | 0.44              |
| 1:1A:1046:A:H62    | 10:1J:4:ASN:HD21  | 1.65                     | 0.44              |
| 1:1A:1410:G:H2'    | 1:1A:1411:U:C6    | 2.53                     | 0.44              |
| 1:1A:1506:U:H2'    | 1:1A:1507:C:C6    | 2.52                     | 0.44              |
| 1:1A:1689:A:H4'    | 35:1a:1475:G:H4'  | 1.99                     | 0.44              |
| 1:1A:1849:G:H2'    | 1:1A:1850:G:H8    | 1.82                     | 0.44              |
| 1:1A:2328:A:H2'    | 1:1A:2329:U:C6    | 2.52                     | 0.44              |
| 3:1D:83:ASP:HB3    | 3:1D:86:ARG:HB2   | 1.98                     | 0.44              |
| 4:1E:55:LYS:HE2    | 4:1E:77:ARG:HA    | 1.99                     | 0.44              |
| 15:1Q:42:THR:HG22  | 15:1Q:93:VAL:HG12 | 2.00                     | 0.44              |
| 35:1a:279:A:H5''   | 35:1a:280:C:O3'   | 2.16                     | 0.44              |
| 35:1a:489:C:H2'    | 35:1a:490:C:C6    | 2.52                     | 0.44              |
| 37:1c:69:THR:HG21  | 37:1c:75:VAL:HG21 | 2.00                     | 0.44              |
| 42:1h:52:GLY:HA3   | 42:1h:56:PRO:HA   | 1.99                     | 0.44              |
| 1:1A:554:U:H2'     | 1:1A:555:G:O4'    | 2.17                     | 0.44              |
| 1:1A:574:A:H2      | 1:1A:2032:G:O2'   | 2.00                     | 0.44              |
| 1:1A:1913:A:C8     | 35:1a:1494:G:H4'  | 2.52                     | 0.44              |
| 1:1A:2893:A:H4'    | 1:1A:2894:G:C4    | 2.52                     | 0.44              |
| 7:1H:68:ARG:HH12   | 7:1H:72:ASN:HD22  | 1.65                     | 0.44              |
| 10:1J:78:GLY:N     | 10:1J:79:PRO:HD2  | 2.31                     | 0.44              |
| 35:1a:216:U:H2'    | 35:1a:217:C:C6    | 2.53                     | 0.44              |
| 35:1a:291:U:H2'    | 35:1a:292:G:C8    | 2.52                     | 0.44              |
| 35:1a:543:U:H2'    | 35:1a:544:G:H8    | 1.83                     | 0.44              |
| 35:1a:765:G:N1     | 35:1a:812:G:O2'   | 2.35                     | 0.44              |
| 35:1a:778:G:H21    | 45:1k:121:ARG:HB2 | 1.81                     | 0.44              |
| 36:1b:35:ASN:HB3   | 36:1b:37:VAL:HG12 | 1.98                     | 0.44              |
| 40:1f:36:ILE:HD12  | 40:1f:64:VAL:HB   | 1.99                     | 0.44              |
| 49:1o:4:THR:O      | 49:1o:7:THR:OG1   | 2.24                     | 0.44              |
| 58:1x:50:G:N2      | 58:1x:65:PSU:C4   | 2.86                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:277:G:H4'    | 1:1A:278:A:N7     | 2.33                     | 0.44              |
| 1:1A:1130:U:O2'   | 1:1A:1131:G:OP1   | 2.29                     | 0.44              |
| 1:1A:1791:A:H5''  | 3:1D:204:LEU:HD12 | 1.99                     | 0.44              |
| 1:1A:2674:G:H2'   | 1:1A:2675:A:C8    | 2.53                     | 0.44              |
| 1:1A:2808:G:H2'   | 1:1A:2890:G:O6    | 2.18                     | 0.44              |
| 12:1N:36:LEU:O    | 12:1N:51:GLY:HA3  | 2.18                     | 0.44              |
| 15:1Q:105:MET:HB2 | 15:1Q:117:PHE:CZ  | 2.53                     | 0.44              |
| 20:1V:79:ARG:O    | 20:1V:81:LYS:N    | 2.44                     | 0.44              |
| 35:1a:67:C:H2'    | 35:1a:68:G:C8     | 2.52                     | 0.44              |
| 35:1a:692:U:H2'   | 35:1a:694:A:OP2   | 2.17                     | 0.44              |
| 35:1a:780:A:H5''  | 45:1k:124:LYS:HD3 | 1.99                     | 0.44              |
| 35:1a:1093:A:C6   | 35:1a:1095:U:H1'  | 2.52                     | 0.44              |
| 35:1a:1280:A:C5   | 44:1j:43:PRO:HD3  | 2.53                     | 0.44              |
| 39:1e:106:ALA:HB3 | 39:1e:111:ARG:HB2 | 1.99                     | 0.44              |
| 45:1k:27:ASN:O    | 45:1k:56:LYS:NZ   | 2.51                     | 0.44              |
| 1:1A:631:A:OP2    | 33:18:22:LYS:NZ   | 2.37                     | 0.44              |
| 1:1A:1061:U:N3    | 11:1K:11:GLN:O    | 2.50                     | 0.44              |
| 1:1A:1361:G:HO2'  | 1:1A:2215:C:HO2'  | 1.62                     | 0.44              |
| 1:1A:1940:U:H4'   | 1:1A:1941:C:O5'   | 2.16                     | 0.44              |
| 2:1B:65:U:H3'     | 2:1B:108:A:H61    | 1.82                     | 0.44              |
| 20:1V:68:ARG:NH1  | 20:1V:90:ARG:HB2  | 2.33                     | 0.44              |
| 23:1Y:3:LYS:HD3   | 23:1Y:82:VAL:HB   | 1.98                     | 0.44              |
| 35:1a:24:U:O3'    | 35:1a:524:G:O2'   | 2.35                     | 0.44              |
| 35:1a:284:C:H2'   | 35:1a:285:C:H6    | 1.81                     | 0.44              |
| 35:1a:1077:G:N2   | 35:1a:1080:A:OP2  | 2.40                     | 0.44              |
| 51:1q:19:SER:HB3  | 51:1q:70:LYS:NZ   | 2.31                     | 0.44              |
| 1:1A:944:C:H5''   | 1:1A:945:A:H5'    | 1.99                     | 0.44              |
| 1:1A:1022:G:H1'   | 1:1A:1023:U:OP2   | 2.18                     | 0.44              |
| 1:1A:1939:5MU:OP1 | 1:1A:2604:PSU:O2' | 2.35                     | 0.44              |
| 1:1A:2032:G:N2    | 4:1E:151:THR:OG1  | 2.50                     | 0.44              |
| 1:1A:2297:A:H8    | 1:1A:2297:A:OP2   | 2.00                     | 0.44              |
| 1:1A:2335:A:H2'   | 1:1A:2336:A:H2'   | 1.99                     | 0.44              |
| 1:1A:2599:G:N7    | 3:1D:234:GLY:HA2  | 2.32                     | 0.44              |
| 1:1A:2624:G:H2'   | 1:1A:2625:G:H8    | 1.83                     | 0.44              |
| 11:1K:131:THR:O   | 11:1K:134:SER:OG  | 2.33                     | 0.44              |
| 14:1P:90:VAL:HB   | 14:1P:122:VAL:HA  | 1.99                     | 0.44              |
| 18:1T:29:VAL:C    | 18:1T:39:LEU:HD12 | 2.43                     | 0.44              |
| 21:1W:6:LYS:HA    | 21:1W:104:THR:HA  | 1.99                     | 0.44              |
| 35:1a:60:A:OP1    | 35:1a:111:G:N2    | 2.47                     | 0.44              |
| 35:1a:579:A:C5'   | 35:1a:728:A:H1'   | 2.48                     | 0.44              |
| 35:1a:599:C:H2'   | 35:1a:600:A:H8    | 1.82                     | 0.44              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 35:1a:968:A:C8    | 35:1a:1062:U:H4'    | 2.53                     | 0.44              |
| 37:1c:173:PRO:HD2 | 37:1c:202:PHE:CD1   | 2.53                     | 0.44              |
| 43:1i:18:VAL:HG22 | 43:1i:64:ILE:HG23   | 2.00                     | 0.44              |
| 1:1A:174:U:H2'    | 1:1A:175:G:C8       | 2.53                     | 0.44              |
| 1:1A:2068:U:H5'   | 1:1A:2069:G7M:OP1   | 2.18                     | 0.44              |
| 3:1D:204:LEU:HD21 | 3:1D:213:ARG:HH21   | 1.83                     | 0.44              |
| 4:1E:33:ARG:HD3   | 4:1E:73:VAL:HB      | 2.00                     | 0.44              |
| 35:1a:513:C:H2'   | 35:1a:514:C:C6      | 2.52                     | 0.44              |
| 35:1a:1147:C:H2'  | 35:1a:1148:U:C6     | 2.53                     | 0.44              |
| 35:1a:1401:G:O5'  | 35:1a:1401:G:H8     | 2.01                     | 0.44              |
| 42:1h:25:THR:HG23 | 42:1h:57:GLU:HB3    | 2.00                     | 0.44              |
| 53:1s:30:LEU:HB2  | 53:1s:48:ILE:HG22   | 1.99                     | 0.44              |
| 1:1A:1612:C:H4'   | 32:17:7:PRO:HD3     | 1.99                     | 0.44              |
| 1:1A:1653:G:O6    | 16:1R:11:ASN:N      | 2.51                     | 0.44              |
| 1:1A:1869:G:H2'   | 1:1A:1871:A:OP1     | 2.17                     | 0.44              |
| 1:1A:1931:U:H2'   | 1:1A:1932:A:H8      | 1.81                     | 0.44              |
| 1:1A:2052:A:O2'   | 4:1E:149:ASN:O      | 2.35                     | 0.44              |
| 1:1A:2772:C:H5'   | 4:1E:173:GLN:HE21   | 1.83                     | 0.44              |
| 2:1B:118:C:H2'    | 2:1B:119:A:C8       | 2.53                     | 0.44              |
| 28:13:10:ARG:NH2  | 28:13:52:PHE:O      | 2.51                     | 0.44              |
| 35:1a:1512:U:H2'  | 35:1a:1513:A:C8     | 2.53                     | 0.44              |
| 35:1a:1517:G:O6   | 35:1a:1518:MA6:H102 | 2.17                     | 0.44              |
| 43:1i:37:TYR:HD2  | 43:1i:38:PHE:HD2    | 1.65                     | 0.44              |
| 45:1k:35:ASP:OD1  | 45:1k:39:ASN:N      | 2.49                     | 0.44              |
| 1:1A:2544:G:H2'   | 1:1A:2545:G:H8      | 1.83                     | 0.44              |
| 2:1B:54:G:N2      | 6:1G:25:MET:SD      | 2.85                     | 0.44              |
| 3:1D:131:MET:HG2  | 3:1D:134:ILE:HD12   | 1.99                     | 0.44              |
| 6:1G:39:VAL:HG23  | 6:1G:149:ARG:HD3    | 2.00                     | 0.44              |
| 6:1G:116:LEU:HD23 | 6:1G:127:TYR:OH     | 2.18                     | 0.44              |
| 15:1Q:50:ARG:HD2  | 15:1Q:65:ILE:HD11   | 2.00                     | 0.44              |
| 33:18:36:ALA:HB3  | 33:18:39:ARG:HG3    | 2.00                     | 0.44              |
| 35:1a:674:G:H2'   | 35:1a:675:A:C8      | 2.53                     | 0.44              |
| 35:1a:775:G:H2'   | 35:1a:776:G:H8      | 1.83                     | 0.44              |
| 35:1a:1499:A:H2'  | 35:1a:1500:A:H8     | 1.83                     | 0.44              |
| 36:1b:203:ASP:OD1 | 36:1b:204:ASP:N     | 2.47                     | 0.44              |
| 43:1i:11:ARG:HA   | 43:1i:105:ARG:NH1   | 2.32                     | 0.44              |
| 54:1t:61:ALA:HB1  | 54:1t:68:LYS:HB3    | 2.00                     | 0.44              |
| 1:1A:780:G:N2     | 3:1D:228:ASP:OD2    | 2.48                     | 0.43              |
| 1:1A:1278:C:H2'   | 1:1A:1279:G:C8      | 2.53                     | 0.43              |
| 1:1A:1307:A:N6    | 1:1A:1606:C:O2'     | 2.51                     | 0.43              |
| 1:1A:1316:U:H2'   | 1:1A:1317:G:C8      | 2.52                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1652:A:N6     | 16:1R:11:ASN:OD1   | 2.49                     | 0.43              |
| 1:1A:1682:G:C5     | 1:1A:1757:A:H1'    | 2.52                     | 0.43              |
| 1:1A:1799:G:P      | 1:1A:1819:A:H61    | 2.41                     | 0.43              |
| 5:1F:102:ARG:HH12  | 5:1F:201:ALA:HB3   | 1.83                     | 0.43              |
| 10:1J:107:GLU:O    | 10:1J:109:LYS:N    | 2.48                     | 0.43              |
| 12:1N:28:LEU:O     | 12:1N:32:LEU:HG    | 2.18                     | 0.43              |
| 22:1X:6:ARG:O      | 22:1X:10:VAL:HG23  | 2.18                     | 0.43              |
| 35:1a:736:C:H2'    | 35:1a:737:C:C6     | 2.53                     | 0.43              |
| 35:1a:769:G:H4'    | 35:1a:1513:A:H4'   | 2.00                     | 0.43              |
| 35:1a:1079:G:H5''  | 39:1e:49:TYR:CZ    | 2.53                     | 0.43              |
| 35:1a:1219:A:H2'   | 35:1a:1220:G:C8    | 2.52                     | 0.43              |
| 36:1b:163:ILE:HD11 | 36:1b:209:VAL:HG11 | 2.00                     | 0.43              |
| 37:1c:58:ARG:CZ    | 37:1c:63:ILE:HD13  | 2.48                     | 0.43              |
| 46:1l:31:GLY:HA2   | 46:1l:56:LEU:HA    | 1.98                     | 0.43              |
| 46:1l:109:ARG:HB2  | 46:1l:118:VAL:HG21 | 2.00                     | 0.43              |
| 1:1A:330:A:H1'     | 1:1A:1210:G:C6     | 2.53                     | 0.43              |
| 1:1A:690:G:H1      | 1:1A:772:C:N4      | 2.10                     | 0.43              |
| 1:1A:956:G:H4'     | 15:1Q:82:MET:HE1   | 2.00                     | 0.43              |
| 1:1A:1382:G:H4'    | 1:1A:1573:G:C2     | 2.52                     | 0.43              |
| 1:1A:1613:G:C2     | 1:1A:1617:C:C2     | 3.05                     | 0.43              |
| 29:14:44:PHE:CD1   | 29:14:45:THR:HG23  | 2.53                     | 0.43              |
| 35:1a:222:C:H2'    | 35:1a:223:A:C8     | 2.52                     | 0.43              |
| 35:1a:375:U:H5''   | 50:1p:70:ARG:HG3   | 2.00                     | 0.43              |
| 35:1a:764:C:H2'    | 35:1a:765:G:C8     | 2.53                     | 0.43              |
| 35:1a:1165:U:H2'   | 35:1a:1166:G:H8    | 1.84                     | 0.43              |
| 35:1a:1254:A:OP2   | 44:1j:45:ARG:NH2   | 2.51                     | 0.43              |
| 35:1a:1413:A:H2    | 35:1a:1487:G:H22   | 1.65                     | 0.43              |
| 39:1e:38:VAL:HG22  | 39:1e:66:ALA:HB1   | 2.00                     | 0.43              |
| 1:1A:82:U:O4       | 1:1A:83:A:N6       | 2.52                     | 0.43              |
| 1:1A:951:C:H2'     | 1:1A:952:G:C8      | 2.53                     | 0.43              |
| 1:1A:1248:G:C6     | 19:1U:2:ARG:HD2    | 2.53                     | 0.43              |
| 1:1A:1419:A:H61    | 1:1A:1494:A:H61    | 1.65                     | 0.43              |
| 1:1A:1681:G:H1'    | 1:1A:1762:A:H2'    | 2.01                     | 0.43              |
| 1:1A:2756:U:H1'    | 1:1A:2757:A:H5''   | 2.01                     | 0.43              |
| 6:1G:35:LEU:HD21   | 6:1G:98:PHE:CZ     | 2.53                     | 0.43              |
| 23:1Y:70:ALA:HB3   | 23:1Y:79:ALA:HB1   | 2.00                     | 0.43              |
| 35:1a:160:A:H2'    | 35:1a:161:A:O4'    | 2.18                     | 0.43              |
| 35:1a:902:G:H2'    | 35:1a:903:G:H8     | 1.84                     | 0.43              |
| 38:1d:57:LYS:NZ    | 38:1d:58:GLN:OE1   | 2.52                     | 0.43              |
| 1:1A:283:G:H1      | 1:1A:357:C:H42     | 1.65                     | 0.43              |
| 1:1A:1268:A:H62    | 1:1A:2012:G:H21    | 1.64                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:1909:C:H2'    | 1:1A:1910:G:H8    | 1.84                     | 0.43              |
| 1:1A:2681:C:OP2    | 4:1E:114:LYS:NZ   | 2.52                     | 0.43              |
| 1:1A:2747:G:H1     | 1:1A:2754:U:H2'   | 1.83                     | 0.43              |
| 1:1A:2755:C:O2'    | 1:1A:2756:U:H2'   | 2.18                     | 0.43              |
| 4:1E:4:LEU:HB2     | 4:1E:101:PHE:CZ   | 2.53                     | 0.43              |
| 4:1E:131:ASP:O     | 4:1E:136:ASN:ND2  | 2.44                     | 0.43              |
| 5:1F:32:VAL:HG21   | 14:1P:3:LEU:HD11  | 2.00                     | 0.43              |
| 6:1G:139:GLU:HA    | 29:14:28:VAL:HG22 | 2.00                     | 0.43              |
| 10:1J:23:LEU:HB3   | 10:1J:87:GLU:OE1  | 2.19                     | 0.43              |
| 13:1O:16:ALA:HB3   | 13:1O:86:LEU:HD11 | 2.01                     | 0.43              |
| 14:1P:14:LYS:O     | 14:1P:16:GLY:N    | 2.51                     | 0.43              |
| 19:1U:95:ALA:O     | 19:1U:99:VAL:HG23 | 2.18                     | 0.43              |
| 21:1W:83:LYS:HG2   | 21:1W:95:ARG:NH1  | 2.34                     | 0.43              |
| 35:1a:240:G:H2'    | 35:1a:241:G:C8    | 2.53                     | 0.43              |
| 35:1a:880:C:H2'    | 35:1a:881:G:C8    | 2.54                     | 0.43              |
| 35:1a:1092:A:OP2   | 41:1g:3:ARG:NH1   | 2.51                     | 0.43              |
| 35:1a:1174:G:H2'   | 35:1a:1175:G:C8   | 2.52                     | 0.43              |
| 37:1c:58:ARG:NH2   | 37:1c:63:ILE:HD13 | 2.34                     | 0.43              |
| 40:1f:15:SER:HA    | 40:1f:18:VAL:HG23 | 2.00                     | 0.43              |
| 46:1l:80:LEU:HD23  | 46:1l:97:VAL:HG11 | 2.01                     | 0.43              |
| 1:1A:107:G:O3'     | 1:1A:293:U:O2'    | 2.36                     | 0.43              |
| 1:1A:110:G:H2'     | 1:1A:111:A:H8     | 1.83                     | 0.43              |
| 1:1A:193:U:H2'     | 1:1A:194:G:H8     | 1.84                     | 0.43              |
| 1:1A:911:A:N1      | 1:1A:2277:G:O2'   | 2.46                     | 0.43              |
| 1:1A:953:G:H2'     | 1:1A:954:G:C8     | 2.48                     | 0.43              |
| 1:1A:1346:G:H2'    | 1:1A:1347:A:H8    | 1.83                     | 0.43              |
| 1:1A:2463:C:H2'    | 1:1A:2464:G:C8    | 2.53                     | 0.43              |
| 13:1O:61:VAL:HG21  | 13:1O:112:PHE:CE1 | 2.53                     | 0.43              |
| 35:1a:374:A:H2'    | 35:1a:375:U:H6    | 1.84                     | 0.43              |
| 35:1a:544:G:OP1    | 38:1d:58:GLN:HG3  | 2.18                     | 0.43              |
| 35:1a:1351:U:O4    | 43:1i:119:LYS:NZ  | 2.51                     | 0.43              |
| 35:1a:1377:A:H4'   | 35:1a:1378:C:H5   | 1.83                     | 0.43              |
| 39:1e:9:GLU:N      | 39:1e:9:GLU:OE1   | 2.51                     | 0.43              |
| 41:1g:12:LEU:HD11  | 43:1i:49:GLN:HE22 | 1.84                     | 0.43              |
| 43:1i:115:VAL:HG21 | 44:1j:62:ARG:HB2  | 1.99                     | 0.43              |
| 1:1A:755:U:H2'     | 1:1A:756:A:C8     | 2.54                     | 0.43              |
| 1:1A:1365:A:OP2    | 26:11:2:ARG:N     | 2.41                     | 0.43              |
| 1:1A:1809:A:H2'    | 1:1A:1810:A:C8    | 2.54                     | 0.43              |
| 1:1A:2787:C:H1'    | 4:1E:63:PRO:HG3   | 2.00                     | 0.43              |
| 4:1E:9:VAL:O       | 4:1E:26:VAL:HB    | 2.18                     | 0.43              |
| 4:1E:133:THR:HG23  | 4:1E:134:HIS:CD2  | 2.53                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:1W:77:ASP:N    | 21:1W:77:ASP:OD1   | 2.50                     | 0.43              |
| 35:1a:25:C:H2'    | 35:1a:26:A:C8      | 2.54                     | 0.43              |
| 35:1a:556:C:H2'   | 35:1a:557:G:C8     | 2.53                     | 0.43              |
| 35:1a:603:U:H2'   | 35:1a:604:G:C8     | 2.53                     | 0.43              |
| 35:1a:779:C:H1'   | 45:1k:121:ARG:HD2  | 1.99                     | 0.43              |
| 35:1a:1099:G:H2'  | 35:1a:1100:C:O4'   | 2.19                     | 0.43              |
| 35:1a:1121:U:H2'  | 35:1a:1122:U:C6    | 2.54                     | 0.43              |
| 35:1a:1157:A:H5'  | 35:1a:1158:C:C5    | 2.54                     | 0.43              |
| 39:1e:37:VAL:HG11 | 39:1e:113:VAL:HG23 | 2.00                     | 0.43              |
| 39:1e:37:VAL:HG21 | 39:1e:136:VAL:HG21 | 2.01                     | 0.43              |
| 46:1l:79:ILE:HG22 | 46:1l:103:CYS:HB2  | 2.01                     | 0.43              |
| 1:1A:20:C:H2'     | 1:1A:21:A:C8       | 2.53                     | 0.43              |
| 1:1A:593:U:H2'    | 1:1A:594:U:C6      | 2.54                     | 0.43              |
| 1:1A:1005:C:H2'   | 1:1A:1006:C:H6     | 1.82                     | 0.43              |
| 1:1A:1318:U:H2'   | 1:1A:1319:C:C6     | 2.54                     | 0.43              |
| 1:1A:1365:A:O5'   | 26:1l:27:ARG:NH2   | 2.49                     | 0.43              |
| 1:1A:2410:G:H2'   | 1:1A:2411:A:O4'    | 2.19                     | 0.43              |
| 4:1E:121:THR:HG23 | 4:1E:162:ALA:HB2   | 2.01                     | 0.43              |
| 4:1E:157:LYS:O    | 12:1N:81:ILE:HB    | 2.17                     | 0.43              |
| 15:1Q:53:MET:HE1  | 15:1Q:117:PHE:CE1  | 2.54                     | 0.43              |
| 15:1Q:136:MET:HB3 | 15:1Q:136:MET:HE2  | 1.63                     | 0.43              |
| 19:1U:20:ALA:HA   | 19:1U:23:TYR:CE2   | 2.53                     | 0.43              |
| 35:1a:454:G:H22   | 35:1a:478:A:H2     | 1.67                     | 0.43              |
| 35:1a:709:U:H2'   | 35:1a:710:G:H8     | 1.83                     | 0.43              |
| 38:1d:1:ALA:O     | 38:1d:67:LEU:HD21  | 2.19                     | 0.43              |
| 43:1i:116:GLY:HA2 | 44:1j:62:ARG:HH12  | 1.83                     | 0.43              |
| 53:1s:49:ALA:HA   | 53:1s:58:PRO:HA    | 2.01                     | 0.43              |
| 54:1t:66:ILE:HG21 | 54:1t:71:ALA:HB2   | 1.99                     | 0.43              |
| 1:1A:281:C:H2'    | 1:1A:282:A:H8      | 1.84                     | 0.43              |
| 1:1A:456:C:H2'    | 22:1X:73:ARG:HH22  | 1.82                     | 0.43              |
| 1:1A:591:U:H1'    | 33:18:1:PRO:H2     | 1.83                     | 0.43              |
| 1:1A:714:U:N3     | 1:1A:717:C:OP2     | 2.50                     | 0.43              |
| 1:1A:1301:A:H2'   | 1:1A:1301:A:N3     | 2.34                     | 0.43              |
| 1:1A:1683:U:H2'   | 1:1A:1684:G:C8     | 2.53                     | 0.43              |
| 1:1A:1790:C:OP2   | 1:1A:1828:G:N1     | 2.47                     | 0.43              |
| 1:1A:2710:C:H2'   | 1:1A:2711:A:C8     | 2.54                     | 0.43              |
| 6:1G:92:GLY:O     | 6:1G:95:MET:HG2    | 2.19                     | 0.43              |
| 7:1H:88:LEU:HG    | 7:1H:161:VAL:HG22  | 2.01                     | 0.43              |
| 13:1O:29:HIS:HE1  | 13:1O:31:ARG:HH12  | 1.63                     | 0.43              |
| 35:1a:377:G:H5'   | 50:1p:5:ARG:NH1    | 2.34                     | 0.43              |
| 35:1a:1061:G:H2'  | 35:1a:1062:U:O4'   | 2.19                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:1a:1230:C:H2'   | 35:1a:1231:G:C8   | 2.53                     | 0.43              |
| 42:1h:10:LEU:HD22  | 42:1h:74:ILE:HG12 | 2.00                     | 0.43              |
| 43:1i:17:ARG:HB2   | 43:1i:65:THR:OG1  | 2.17                     | 0.43              |
| 43:1i:30:ASN:C     | 43:1i:32:ARG:H    | 2.27                     | 0.43              |
| 43:1i:80:HIS:CD2   | 43:1i:105:ARG:HA  | 2.53                     | 0.43              |
| 1:1A:155:A:H2'     | 1:1A:156:A:C8     | 2.54                     | 0.43              |
| 1:1A:190:A:H5''    | 1:1A:204:A:N6     | 2.30                     | 0.43              |
| 1:1A:209:C:H4'     | 1:1A:681:G:H4'    | 1.99                     | 0.43              |
| 1:1A:603:A:N6      | 1:1A:655:A:O4'    | 2.51                     | 0.43              |
| 1:1A:831:G:O2'     | 14:1P:38:GLN:OE1  | 2.35                     | 0.43              |
| 1:1A:1340:U:H4'    | 1:1A:1394:U:O2'   | 2.19                     | 0.43              |
| 1:1A:1491:G:H2'    | 1:1A:1492:G:C8    | 2.53                     | 0.43              |
| 1:1A:1595:C:H2'    | 1:1A:1596:A:C8    | 2.54                     | 0.43              |
| 1:1A:1882:U:H2'    | 1:1A:1883:U:H6    | 1.84                     | 0.43              |
| 1:1A:2061:G:H2'    | 1:1A:2501:C:O2'   | 2.19                     | 0.43              |
| 1:1A:2353:G:H2'    | 1:1A:2354:C:O4'   | 2.19                     | 0.43              |
| 1:1A:2630:G:H2'    | 1:1A:2631:G:C8    | 2.54                     | 0.43              |
| 3:1D:209:ALA:HA    | 3:1D:212:TRP:CZ2  | 2.54                     | 0.43              |
| 10:1J:26:VAL:HG21  | 10:1J:114:GLU:HG2 | 2.01                     | 0.43              |
| 10:1J:79:PRO:O     | 10:1J:80:THR:OG1  | 2.30                     | 0.43              |
| 26:11:37:PHE:HZ    | 26:11:55:MET:HG2  | 1.84                     | 0.43              |
| 32:17:34:ARG:HB2   | 32:17:42:LEU:HD12 | 2.01                     | 0.43              |
| 35:1a:1056:U:H2'   | 35:1a:1057:G:H8   | 1.84                     | 0.43              |
| 42:1h:94:VAL:HG23  | 42:1h:101:ALA:HB2 | 2.00                     | 0.43              |
| 43:1i:118:ARG:HH21 | 43:1i:122:ARG:HG2 | 1.84                     | 0.43              |
| 1:1A:16:C:H2'      | 1:1A:17:G:H8      | 1.84                     | 0.43              |
| 1:1A:221:A:N1      | 1:1A:265:A:O2'    | 2.48                     | 0.43              |
| 1:1A:537:G:H4'     | 12:1N:5:THR:HG21  | 2.00                     | 0.43              |
| 1:1A:832:U:P       | 14:1P:38:GLN:H    | 2.41                     | 0.43              |
| 1:1A:1020:A:H4'    | 1:1A:1021:A:O5'   | 2.18                     | 0.43              |
| 1:1A:1213:A:N6     | 1:1A:1236:G:H1'   | 2.34                     | 0.43              |
| 1:1A:1565:C:O2'    | 1:1A:1566:A:H8    | 2.02                     | 0.43              |
| 1:1A:1834:U:O2'    | 1:1A:1969:A:H3'   | 2.18                     | 0.43              |
| 1:1A:2073:C:O2'    | 1:1A:2598:A:O2'   | 2.32                     | 0.43              |
| 1:1A:2591:C:C2     | 1:1A:2592:G:C8    | 3.07                     | 0.43              |
| 1:1A:2630:G:H2'    | 1:1A:2631:G:H8    | 1.84                     | 0.43              |
| 16:1R:49:GLU:HB2   | 16:1R:50:PRO:HD3  | 2.00                     | 0.43              |
| 21:1W:88:ARG:HD2   | 21:1W:88:ARG:HA   | 1.76                     | 0.43              |
| 28:13:43:ILE:O     | 28:13:47:ILE:HG13 | 2.19                     | 0.43              |
| 35:1a:319:G:H2'    | 35:1a:320:A:C8    | 2.53                     | 0.43              |
| 35:1a:946:A:H2'    | 35:1a:947:G:C8    | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:1c:84:GLU:HG3  | 37:1c:87:ARG:HH22 | 1.84                     | 0.43              |
| 50:1p:23:ASP:HB3  | 50:1p:26:ASN:ND2  | 2.34                     | 0.43              |
| 1:1A:404:A:H1'    | 1:1A:406:G:C4     | 2.54                     | 0.42              |
| 1:1A:934:U:H2'    | 1:1A:935:C:C6     | 2.54                     | 0.42              |
| 1:1A:1183:U:H2'   | 1:1A:1184:U:C6    | 2.53                     | 0.42              |
| 1:1A:2140:G:H2'   | 1:1A:2141:G:C8    | 2.53                     | 0.42              |
| 1:1A:2200:C:H2'   | 1:1A:2201:G:H8    | 1.83                     | 0.42              |
| 1:1A:2437:G:O2'   | 1:1A:2599:G:H4'   | 2.19                     | 0.42              |
| 12:1N:74:TYR:HE2  | 12:1N:89:PHE:HD1  | 1.68                     | 0.42              |
| 16:1R:48:VAL:O    | 16:1R:52:ILE:HG13 | 2.19                     | 0.42              |
| 21:1W:84:ARG:HB2  | 21:1W:96:ILE:HG13 | 2.01                     | 0.42              |
| 29:14:56:ARG:NH2  | 47:1m:78:ARG:HD2  | 2.34                     | 0.42              |
| 35:1a:234:C:O2'   | 51:1q:71:SER:OG   | 2.35                     | 0.42              |
| 35:1a:309:A:O2'   | 35:1a:607:A:N1    | 2.52                     | 0.42              |
| 35:1a:1026:G:H2'  | 35:1a:1027:C:C6   | 2.54                     | 0.42              |
| 36:1b:41:ASN:HD22 | 36:1b:44:LYS:HG2  | 1.84                     | 0.42              |
| 40:1f:45:ARG:HH22 | 52:1r:25:ILE:HD11 | 1.84                     | 0.42              |
| 48:1n:85:ARG:O    | 48:1n:89:MET:HG2  | 2.19                     | 0.42              |
| 53:1s:39:ILE:HB   | 53:1s:66:VAL:O    | 2.18                     | 0.42              |
| 1:1A:27:G:N2      | 1:1A:512:G:H1'    | 2.33                     | 0.42              |
| 1:1A:1336:A:H2'   | 1:1A:1337:G:C8    | 2.54                     | 0.42              |
| 1:1A:1539:U:H2'   | 1:1A:1540:G:C8    | 2.53                     | 0.42              |
| 1:1A:1565:C:O2'   | 1:1A:1566:A:H2'   | 2.19                     | 0.42              |
| 1:1A:2137:U:H2'   | 1:1A:2138:G:C8    | 2.54                     | 0.42              |
| 1:1A:2539:C:H5'   | 34:19:3:VAL:HG11  | 2.01                     | 0.42              |
| 6:1G:137:PHE:HA   | 6:1G:138:PRO:HD3  | 1.91                     | 0.42              |
| 9:1I:9:VAL:HG12   | 9:1I:11:ASN:H     | 1.82                     | 0.42              |
| 16:1R:69:ARG:O    | 16:1R:71:ARG:N    | 2.47                     | 0.42              |
| 25:10:42:HIS:CD2  | 25:10:73:ARG:HD3  | 2.54                     | 0.42              |
| 26:11:4:CYS:HB3   | 26:11:8:GLY:H     | 1.84                     | 0.42              |
| 35:1a:10:A:H2'    | 35:1a:11:G:H8     | 1.85                     | 0.42              |
| 35:1a:51:A:N1     | 35:1a:314:C:O2'   | 2.43                     | 0.42              |
| 35:1a:295:C:C4    | 35:1a:296:U:C4    | 3.07                     | 0.42              |
| 35:1a:377:G:H5'   | 50:1p:5:ARG:HH12  | 1.84                     | 0.42              |
| 35:1a:1108:G:H5'  | 37:1c:175:HIS:CE1 | 2.54                     | 0.42              |
| 35:1a:1405:G:C2   | 35:1a:1406:U:C4   | 3.07                     | 0.42              |
| 35:1a:1475:G:H2'  | 35:1a:1476:A:H8   | 1.83                     | 0.42              |
| 37:1c:56:ILE:HG22 | 37:1c:63:ILE:HD11 | 2.01                     | 0.42              |
| 45:1k:24:ALA:HB1  | 45:1k:29:THR:HG22 | 2.01                     | 0.42              |
| 47:1m:53:ASP:OD1  | 47:1m:54:THR:N    | 2.52                     | 0.42              |
| 53:1s:8:PRO:HB3   | 53:1s:38:THR:HG21 | 2.01                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:438:G:H2'     | 1:1A:439:A:H8     | 1.84                     | 0.42              |
| 1:1A:596:U:H2'     | 1:1A:597:G:H8     | 1.84                     | 0.42              |
| 1:1A:643:A:N1      | 1:1A:2369:A:O2'   | 2.49                     | 0.42              |
| 1:1A:671:C:H2'     | 1:1A:672:C:C6     | 2.55                     | 0.42              |
| 1:1A:776:G:N2      | 1:1A:2072:C:H5'   | 2.16                     | 0.42              |
| 1:1A:2746:U:H1'    | 7:1H:138:GLN:HE22 | 1.85                     | 0.42              |
| 1:1A:2872:A:H2'    | 1:1A:2873:A:C8    | 2.54                     | 0.42              |
| 5:1F:151:GLY:N     | 5:1F:192:ALA:HB2  | 2.33                     | 0.42              |
| 13:1O:104:THR:HG22 | 13:1O:106:GLU:H   | 1.84                     | 0.42              |
| 21:1W:4:ILE:HD12   | 21:1W:6:LYS:HE3   | 2.01                     | 0.42              |
| 35:1a:161:A:H2'    | 35:1a:162:A:O4'   | 2.19                     | 0.42              |
| 35:1a:545:C:P      | 38:1d:61:ARG:HH12 | 2.42                     | 0.42              |
| 35:1a:1417:G:C6    | 35:1a:1482:G:C6   | 3.07                     | 0.42              |
| 39:1e:47:PHE:O     | 39:1e:69:ASN:ND2  | 2.52                     | 0.42              |
| 41:1g:46:LEU:HD23  | 41:1g:57:GLU:HB3  | 2.01                     | 0.42              |
| 50:1p:36:VAL:HG23  | 50:1p:53:ASP:HB3  | 2.01                     | 0.42              |
| 1:1A:375:G:H2'     | 1:1A:376:G:C8     | 2.54                     | 0.42              |
| 1:1A:402:A:H2'     | 1:1A:403:U:O4'    | 2.19                     | 0.42              |
| 1:1A:563:A:N6      | 1:1A:577:G:O6     | 2.52                     | 0.42              |
| 1:1A:1272:A:O2'    | 1:1A:1274:A:OP1   | 2.29                     | 0.42              |
| 1:1A:1592:C:H2'    | 1:1A:1593:A:C8    | 2.55                     | 0.42              |
| 1:1A:1822:C:H2'    | 1:1A:1823:G:C8    | 2.55                     | 0.42              |
| 1:1A:1833:C:O2'    | 1:1A:1969:A:N1    | 2.37                     | 0.42              |
| 1:1A:2052:A:H2'    | 1:1A:2053:G:C8    | 2.54                     | 0.42              |
| 1:1A:2286:G:H4'    | 1:1A:2287:A:O4'   | 2.19                     | 0.42              |
| 1:1A:2687:U:H2'    | 1:1A:2688:G:O4'   | 2.20                     | 0.42              |
| 1:1A:2884:U:H2'    | 1:1A:2885:G:C8    | 2.54                     | 0.42              |
| 3:1D:222:THR:O     | 3:1D:232:GLY:HA2  | 2.19                     | 0.42              |
| 35:1a:376:G:H4'    | 50:1p:5:ARG:HD2   | 2.00                     | 0.42              |
| 35:1a:408:A:P      | 38:1d:7:LYS:HE2   | 2.60                     | 0.42              |
| 35:1a:476:U:H2'    | 35:1a:477:C:C6    | 2.54                     | 0.42              |
| 38:1d:56:GLU:HG2   | 38:1d:198:LEU:HB2 | 2.00                     | 0.42              |
| 38:1d:63:ILE:O     | 38:1d:110:ARG:NE  | 2.52                     | 0.42              |
| 58:1x:29:C:H2'     | 58:1x:30:C:H6     | 1.84                     | 0.42              |
| 1:1A:2347:C:H2'    | 1:1A:2348:U:C6    | 2.54                     | 0.42              |
| 3:1D:7:PRO:HB3     | 3:1D:13:ARG:HG3   | 2.00                     | 0.42              |
| 4:1E:2:ILE:HD13    | 4:1E:48:ILE:HD11  | 2.01                     | 0.42              |
| 9:1I:25:TYR:O      | 9:1I:29:PHE:HB3   | 2.19                     | 0.42              |
| 14:1P:62:PRO:HG2   | 33:18:24:LYS:HB3  | 2.02                     | 0.42              |
| 15:1Q:50:ARG:CD    | 15:1Q:65:ILE:HD11 | 2.50                     | 0.42              |
| 21:1W:44:ALA:HA    | 21:1W:47:VAL:HG12 | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:1a:54:C:H41    | 35:1a:352:C:H3'   | 1.84                     | 0.42              |
| 35:1a:231:U:H2'   | 35:1a:232:G:H8    | 1.84                     | 0.42              |
| 35:1a:508:U:H1'   | 35:1a:509:A:N7    | 2.35                     | 0.42              |
| 35:1a:877:G:H2'   | 35:1a:878:A:C8    | 2.52                     | 0.42              |
| 37:1c:113:LYS:HD3 | 37:1c:184:ASN:ND2 | 2.34                     | 0.42              |
| 38:1d:167:PRO:HB3 | 38:1d:169:TRP:CE2 | 2.54                     | 0.42              |
| 46:1l:70:GLY:O    | 46:1l:98:ARG:NH1  | 2.53                     | 0.42              |
| 56:1v:26:G:N1     | 57:1w:442:TRP:HH2 | 2.18                     | 0.42              |
| 58:1x:5:U:H3      | 58:1x:68:G:H1     | 1.66                     | 0.42              |
| 1:1A:52:A:H8      | 1:1A:52:A:OP2     | 2.02                     | 0.42              |
| 1:1A:288:U:H2'    | 1:1A:289:G:H8     | 1.85                     | 0.42              |
| 1:1A:326:G:H2'    | 1:1A:327:G:H8     | 1.84                     | 0.42              |
| 1:1A:668:A:N3     | 1:1A:670:A:N6     | 2.68                     | 0.42              |
| 1:1A:858:G:O2'    | 1:1A:859:G:OP1    | 2.33                     | 0.42              |
| 1:1A:1020:A:H1'   | 1:1A:1021:A:OP2   | 2.20                     | 0.42              |
| 1:1A:1442:U:H2'   | 1:1A:1443:U:C6    | 2.54                     | 0.42              |
| 1:1A:1744:A:H3'   | 1:1A:1745:A:H8    | 1.83                     | 0.42              |
| 1:1A:2103:C:H2'   | 1:1A:2104:C:C6    | 2.55                     | 0.42              |
| 1:1A:2192:U:H2'   | 1:1A:2193:G:C8    | 2.55                     | 0.42              |
| 5:1F:70:SER:HB2   | 5:1F:78:TRP:HZ2   | 1.85                     | 0.42              |
| 6:1G:127:TYR:HE2  | 6:1G:129:MET:HE2  | 1.83                     | 0.42              |
| 9:1I:30:LEU:HB3   | 9:1I:36:ALA:HB3   | 2.01                     | 0.42              |
| 10:1J:18:VAL:HG11 | 10:1J:70:GLU:HB3  | 2.00                     | 0.42              |
| 30:15:42:ILE:HG22 | 30:15:48:TYR:HB2  | 2.01                     | 0.42              |
| 35:1a:301:G:H2'   | 35:1a:302:G:C8    | 2.54                     | 0.42              |
| 35:1a:332:G:C6    | 35:1a:333:U:C4    | 3.08                     | 0.42              |
| 35:1a:772:U:H2'   | 35:1a:773:G:C8    | 2.54                     | 0.42              |
| 43:1i:64:ILE:HD13 | 43:1i:78:ILE:HG21 | 2.01                     | 0.42              |
| 1:1A:929:U:H4'    | 28:13:37:ARG:NH2  | 2.35                     | 0.42              |
| 1:1A:1326:U:H2'   | 1:1A:1327:A:H8    | 1.85                     | 0.42              |
| 1:1A:1549:A:O3'   | 1:1A:1740:G:N2    | 2.53                     | 0.42              |
| 1:1A:1675:C:H2'   | 1:1A:1676:A:O4'   | 2.18                     | 0.42              |
| 5:1F:131:THR:HG22 | 5:1F:160:ALA:HA   | 2.02                     | 0.42              |
| 6:1G:7:TYR:HB2    | 6:1G:172:PHE:HZ   | 1.84                     | 0.42              |
| 12:1N:64:VAL:HB   | 12:1N:68:LYS:HE3  | 2.01                     | 0.42              |
| 16:1R:59:SER:OG   | 16:1R:62:ASN:OD1  | 2.24                     | 0.42              |
| 23:1Y:36:GLU:HA   | 23:1Y:61:GLU:HG2  | 2.00                     | 0.42              |
| 31:16:7:LYS:HA    | 31:16:23:THR:HA   | 2.00                     | 0.42              |
| 34:19:7:VAL:HG11  | 34:19:37:GLN:O    | 2.20                     | 0.42              |
| 35:1a:1347:G:C5'  | 43:1i:108:ARG:HB2 | 2.49                     | 0.42              |
| 35:1a:1396:A:H4'  | 35:1a:1398:A:H1'  | 2.02                     | 0.42              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 35:1a:1417:G:N2     | 35:1a:1482:G:H2'  | 2.34                     | 0.42              |
| 46:1l:20:VAL:O      | 46:1l:22:ALA:N    | 2.53                     | 0.42              |
| 1:1A:262:A:H2'      | 1:1A:263:G:O4'    | 2.19                     | 0.42              |
| 1:1A:381:G:H2'      | 1:1A:382:A:C8     | 2.55                     | 0.42              |
| 1:1A:970:U:C2       | 1:1A:971:G:C8     | 3.08                     | 0.42              |
| 26:11:39:VAL:HG22   | 26:11:63:ILE:HG12 | 2.02                     | 0.42              |
| 35:1a:426:U:H4'     | 38:1d:39:GLN:HA   | 2.02                     | 0.42              |
| 35:1a:765:G:N2      | 35:1a:813:U:H5    | 2.16                     | 0.42              |
| 35:1a:1281:C:P      | 35:1a:1282:C:H41  | 2.43                     | 0.42              |
| 35:1a:1347:G:N2     | 35:1a:1374:A:OP2  | 2.45                     | 0.42              |
| 41:1g:75:LYS:HE3    | 41:1g:88:VAL:HG11 | 2.02                     | 0.42              |
| 53:1s:10:ILE:HG21   | 53:1s:40:PHE:CE2  | 2.54                     | 0.42              |
| 58:1x:15:G:H2'      | 58:1x:59:G:H22    | 1.85                     | 0.42              |
| 1:1A:468:G:O6       | 32:17:39:ARG:NH2  | 2.47                     | 0.42              |
| 1:1A:714:U:H5''     | 49:1o:88:ARG:HH21 | 1.83                     | 0.42              |
| 1:1A:2008:C:H2'     | 1:1A:2009:A:C8    | 2.55                     | 0.42              |
| 1:1A:2020:A:N6      | 1:1A:2034:U:H3    | 2.16                     | 0.42              |
| 3:1D:43:ASN:HB3     | 3:1D:49:THR:HG21  | 2.01                     | 0.42              |
| 5:1F:147:LEU:HB2    | 5:1F:183:PHE:CD2  | 2.55                     | 0.42              |
| 9:1I:93:SER:HB3     | 9:1I:121:VAL:HB   | 2.01                     | 0.42              |
| 17:1S:51:ALA:HB3    | 17:1S:78:VAL:HG22 | 2.01                     | 0.42              |
| 23:1Y:23:LYS:O      | 23:1Y:35:VAL:HG13 | 2.20                     | 0.42              |
| 33:18:30:HIS:ND1    | 33:18:31:ILE:HG13 | 2.35                     | 0.42              |
| 35:1a:349:A:H2'     | 35:1a:350:G:C8    | 2.54                     | 0.42              |
| 35:1a:1118:U:H2'    | 35:1a:1119:C:C6   | 2.55                     | 0.42              |
| 35:1a:1173:U:H2'    | 35:1a:1174:G:C8   | 2.55                     | 0.42              |
| 35:1a:1300:G:O2'    | 35:1a:1301:U:O5'  | 2.37                     | 0.42              |
| 39:1e:96:GLN:HB3    | 39:1e:123:LEU:HB2 | 2.01                     | 0.42              |
| 50:1p:59:HIS:O      | 50:1p:63:GLN:HG2  | 2.20                     | 0.42              |
| 58:1x:50:G:C2       | 58:1x:51:U:C2     | 3.08                     | 0.42              |
| 1:1A:300:A:P        | 23:1Y:81:ARG:HH12 | 2.42                     | 0.42              |
| 1:1A:2619:C:H2'     | 1:1A:2620:C:H6    | 1.84                     | 0.42              |
| 12:1N:69:ARG:HA     | 12:1N:89:PHE:HD2  | 1.85                     | 0.42              |
| 35:1a:60:A:OP1      | 35:1a:331:G:N1    | 2.42                     | 0.42              |
| 35:1a:765:G:C6      | 35:1a:812:G:C4    | 3.08                     | 0.42              |
| 35:1a:1011:C:H2'    | 35:1a:1012:A:C8   | 2.55                     | 0.42              |
| 35:1a:1407:5MC:HM53 | 35:1a:1408:A:H62  | 1.85                     | 0.42              |
| 54:1t:14:GLU:OE1    | 54:1t:17:ARG:NE   | 2.38                     | 0.42              |
| 1:1A:674:G:H1       | 1:1A:806:C:H42    | 1.67                     | 0.41              |
| 1:1A:747:5MU:H73    | 1:1A:2613:U:C5    | 2.55                     | 0.41              |
| 1:1A:774:G:N2       | 1:1A:787:C:O2'    | 2.53                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:873:C:H2'    | 1:1A:874:G:C8      | 2.54                     | 0.41              |
| 1:1A:1801:A:H5''  | 1:1A:2203:U:H2'    | 2.02                     | 0.41              |
| 5:1F:148:ILE:HB   | 5:1F:169:VAL:HG22  | 2.00                     | 0.41              |
| 13:1O:41:ILE:HG13 | 13:1O:58:LEU:O     | 2.20                     | 0.41              |
| 15:1Q:53:MET:HB3  | 15:1Q:120:ALA:HB2  | 2.01                     | 0.41              |
| 19:1U:97:ILE:HG22 | 19:1U:105:PHE:HB2  | 2.02                     | 0.41              |
| 35:1a:78:A:H2'    | 35:1a:79:G:O4'     | 2.20                     | 0.41              |
| 35:1a:1297:G:H1'  | 35:1a:1298:U:OP2   | 2.20                     | 0.41              |
| 37:1c:59:PRO:HB3  | 44:1j:94:ALA:HB2   | 2.02                     | 0.41              |
| 45:1k:70:ALA:HB1  | 45:1k:104:PHE:HE2  | 1.85                     | 0.41              |
| 48:1n:26:GLU:HB2  | 48:1n:30:ILE:HD12  | 2.01                     | 0.41              |
| 1:1A:672:C:H5     | 14:1P:42:SER:HB2   | 1.85                     | 0.41              |
| 1:1A:806:C:H3'    | 14:1P:41:ARG:HH11  | 1.85                     | 0.41              |
| 1:1A:848:C:H2'    | 1:1A:849:A:C8      | 2.56                     | 0.41              |
| 1:1A:1054:A:OP1   | 10:1J:31:ARG:NH1   | 2.45                     | 0.41              |
| 1:1A:1265:A:N1    | 1:1A:2013:A:H5''   | 2.35                     | 0.41              |
| 1:1A:1407:G:H2'   | 1:1A:1408:G:C8     | 2.54                     | 0.41              |
| 1:1A:1428:C:C4    | 1:1A:1569:A:H5''   | 2.55                     | 0.41              |
| 1:1A:1589:U:H2'   | 1:1A:1590:A:C8     | 2.55                     | 0.41              |
| 1:1A:1909:C:H2'   | 1:1A:1910:G:C8     | 2.55                     | 0.41              |
| 1:1A:2427:C:H5'   | 1:1A:2429:G:H5'    | 2.02                     | 0.41              |
| 1:1A:2544:G:H2'   | 1:1A:2545:G:C8     | 2.55                     | 0.41              |
| 4:1E:136:ASN:OD1  | 4:1E:137:SER:N     | 2.53                     | 0.41              |
| 12:1N:17:VAL:HG22 | 12:1N:55:ILE:HB    | 2.02                     | 0.41              |
| 12:1N:44:TYR:O    | 19:1U:63:ARG:NE    | 2.52                     | 0.41              |
| 22:1X:80:TRP:CZ3  | 22:1X:82:LYS:HD2   | 2.55                     | 0.41              |
| 35:1a:109:A:C6    | 35:1a:327:A:C6     | 3.08                     | 0.41              |
| 35:1a:668:G:H2'   | 35:1a:669:G:C8     | 2.55                     | 0.41              |
| 35:1a:883:C:H2'   | 35:1a:884:U:C6     | 2.55                     | 0.41              |
| 35:1a:1405:G:H2'  | 35:1a:1406:U:C6    | 2.55                     | 0.41              |
| 38:1d:169:TRP:HZ3 | 38:1d:189:ASP:HB3  | 1.85                     | 0.41              |
| 39:1e:149:PRO:HA  | 39:1e:152:VAL:HG22 | 2.01                     | 0.41              |
| 40:1f:51:ILE:HD13 | 40:1f:86:ARG:NH1   | 2.35                     | 0.41              |
| 40:1f:74:LEU:O    | 40:1f:77:THR:OG1   | 2.30                     | 0.41              |
| 43:1i:83:THR:HG21 | 43:1i:102:PHE:HB3  | 2.03                     | 0.41              |
| 44:1j:68:ARG:HB3  | 44:1j:70:HIS:CE1   | 2.55                     | 0.41              |
| 51:1q:51:GLU:OE1  | 51:1q:51:GLU:N     | 2.44                     | 0.41              |
| 58:1x:66:C:O5'    | 58:1x:66:C:H6      | 2.03                     | 0.41              |
| 1:1A:121:G:H4'    | 1:1A:149:A:H5'     | 2.02                     | 0.41              |
| 1:1A:224:U:O4     | 1:1A:419:U:O2'     | 2.38                     | 0.41              |
| 1:1A:279:A:N6     | 1:1A:361:G:H1'     | 2.35                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:281:C:H2'    | 1:1A:282:A:C8     | 2.54                     | 0.41              |
| 1:1A:729:G:H3'    | 1:1A:729:G:N3     | 2.35                     | 0.41              |
| 1:1A:1320:C:O2'   | 1:1A:1321:A:H5''  | 2.21                     | 0.41              |
| 1:1A:1592:C:H2'   | 1:1A:1593:A:H8    | 1.84                     | 0.41              |
| 1:1A:2430:A:H5'   | 1:1A:2431:U:OP2   | 2.20                     | 0.41              |
| 1:1A:2466:C:OP1   | 34:19:4:ARG:HB3   | 2.20                     | 0.41              |
| 1:1A:2619:C:H2'   | 1:1A:2620:C:C6    | 2.55                     | 0.41              |
| 1:1A:2674:G:H2'   | 1:1A:2675:A:H8    | 1.85                     | 0.41              |
| 1:1A:2863:C:H2'   | 1:1A:2864:G:H8    | 1.85                     | 0.41              |
| 3:1D:60:ALA:HB3   | 3:1D:62:ARG:HH12  | 1.85                     | 0.41              |
| 10:1J:25:ALA:HB2  | 10:1J:96:PHE:CD1  | 2.55                     | 0.41              |
| 12:1N:37:ARG:HD3  | 12:1N:39:LYS:HD2  | 2.01                     | 0.41              |
| 23:1Y:32:LYS:HB3  | 23:1Y:63:ALA:HB1  | 2.02                     | 0.41              |
| 24:1Z:4:ILE:HD13  | 24:1Z:47:VAL:HG22 | 2.02                     | 0.41              |
| 24:1Z:10:LYS:HG3  | 24:1Z:11:GLU:HG3  | 2.02                     | 0.41              |
| 35:1a:243:A:H4'   | 35:1a:244:U:H3'   | 2.01                     | 0.41              |
| 35:1a:596:A:H61   | 35:1a:644:U:H3    | 1.68                     | 0.41              |
| 35:1a:677:U:H2'   | 35:1a:678:U:C6    | 2.56                     | 0.41              |
| 36:1b:42:LEU:O    | 36:1b:46:VAL:HG23 | 2.20                     | 0.41              |
| 37:1c:33:ASP:O    | 37:1c:37:LYS:HG2  | 2.20                     | 0.41              |
| 38:1d:9:LYS:HG3   | 38:1d:12:ARG:HH21 | 1.86                     | 0.41              |
| 39:1e:92:ARG:HB2  | 39:1e:127:TYR:HB2 | 2.01                     | 0.41              |
| 45:1k:108:ASN:HB2 | 55:1u:5:VAL:O     | 2.19                     | 0.41              |
| 1:1A:145:C:H2'    | 1:1A:146:A:C8     | 2.55                     | 0.41              |
| 1:1A:185:G:H2'    | 1:1A:186:G:C8     | 2.55                     | 0.41              |
| 1:1A:196:A:N1     | 14:1P:50:PHE:HZ   | 2.18                     | 0.41              |
| 1:1A:764:A:H2     | 3:1D:217:PRO:HG2  | 1.85                     | 0.41              |
| 1:1A:952:G:O2'    | 1:1A:2267:A:H1'   | 2.21                     | 0.41              |
| 1:1A:1013:C:H2'   | 1:1A:1014:A:C8    | 2.53                     | 0.41              |
| 1:1A:2408:U:H2'   | 1:1A:2409:G:H8    | 1.85                     | 0.41              |
| 5:1F:40:ARG:HG2   | 5:1F:42:GLY:H     | 1.84                     | 0.41              |
| 10:1J:28:ALA:H    | 10:1J:110:ALA:HA  | 1.85                     | 0.41              |
| 14:1P:62:PRO:HB2  | 33:18:29:ARG:NH1  | 2.25                     | 0.41              |
| 14:1P:96:LYS:HG3  | 14:1P:102:GLY:O   | 2.20                     | 0.41              |
| 35:1a:98:A:H2'    | 35:1a:99:C:C6     | 2.55                     | 0.41              |
| 35:1a:231:U:H2'   | 35:1a:232:G:C8    | 2.55                     | 0.41              |
| 35:1a:374:A:H2'   | 35:1a:375:U:C6    | 2.56                     | 0.41              |
| 35:1a:880:C:H2'   | 35:1a:881:G:H8    | 1.85                     | 0.41              |
| 35:1a:1269:A:O2'  | 35:1a:1325:C:O2'  | 2.16                     | 0.41              |
| 41:1g:78:ARG:HB3  | 41:1g:83:THR:HA   | 2.03                     | 0.41              |
| 1:1A:184:C:H2'    | 1:1A:185:G:C8     | 2.56                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:246:C:N4      | 33:18:7:ARG:HG3   | 2.36                     | 0.41              |
| 1:1A:964:C:O2'     | 1:1A:2273:A:N3    | 2.53                     | 0.41              |
| 1:1A:974:G:H1'     | 1:1A:975:A:C8     | 2.56                     | 0.41              |
| 1:1A:1346:G:H2'    | 1:1A:1347:A:C8    | 2.55                     | 0.41              |
| 1:1A:2004:G:H2'    | 1:1A:2005:A:O4'   | 2.20                     | 0.41              |
| 1:1A:2143:C:H2'    | 1:1A:2144:G:C8    | 2.55                     | 0.41              |
| 1:1A:2291:U:H2'    | 1:1A:2292:U:C6    | 2.55                     | 0.41              |
| 1:1A:2676:C:H2'    | 1:1A:2677:G:C8    | 2.54                     | 0.41              |
| 1:1A:2788:C:H2'    | 1:1A:2789:C:C6    | 2.55                     | 0.41              |
| 3:1D:28:PRO:HG3    | 3:1D:62:ARG:NH2   | 2.35                     | 0.41              |
| 5:1F:3:LEU:HD21    | 5:1F:19:PHE:CE2   | 2.55                     | 0.41              |
| 14:1P:64:PHE:CZ    | 33:18:23:HIS:HA   | 2.56                     | 0.41              |
| 15:1Q:40:ARG:H     | 15:1Q:40:ARG:HG2  | 1.40                     | 0.41              |
| 15:1Q:71:LYS:HB3   | 15:1Q:93:VAL:O    | 2.20                     | 0.41              |
| 24:1Z:56:PHE:CE1   | 24:1Z:61:LEU:HD21 | 2.56                     | 0.41              |
| 28:13:46:MET:O     | 28:13:50:VAL:HG22 | 2.21                     | 0.41              |
| 35:1a:481:G:O2'    | 35:1a:483:C:N4    | 2.53                     | 0.41              |
| 35:1a:563:A:H61    | 35:1a:884:U:H3    | 1.69                     | 0.41              |
| 35:1a:714:G:C6     | 35:1a:715:A:C6    | 3.09                     | 0.41              |
| 35:1a:782:A:H4'    | 35:1a:1515:G:O4'  | 2.20                     | 0.41              |
| 35:1a:999:C:H2'    | 35:1a:1000:A:C8   | 2.54                     | 0.41              |
| 1:1A:33:C:O2       | 1:1A:447:A:N6     | 2.53                     | 0.41              |
| 1:1A:79:C:O2'      | 1:1A:346:A:N3     | 2.45                     | 0.41              |
| 1:1A:141:G:N2      | 1:1A:142:A:N3     | 2.69                     | 0.41              |
| 1:1A:310:A:H2'     | 1:1A:311:A:H5''   | 2.02                     | 0.41              |
| 1:1A:322:A:H5'     | 1:1A:340:A:H1'    | 2.03                     | 0.41              |
| 1:1A:580:U:H2'     | 1:1A:581:C:C6     | 2.56                     | 0.41              |
| 1:1A:739:A:N3      | 1:1A:740:C:N4     | 2.69                     | 0.41              |
| 1:1A:768:G:C6      | 1:1A:769:U:C4     | 3.09                     | 0.41              |
| 1:1A:841:G:C2      | 1:1A:842:U:C2     | 3.09                     | 0.41              |
| 1:1A:2048:G:H2'    | 1:1A:2049:G:O4'   | 2.21                     | 0.41              |
| 4:1E:85:ALA:C      | 4:1E:87:GLY:H     | 2.28                     | 0.41              |
| 12:1N:24:THR:HB    | 12:1N:27:ARG:HB2  | 2.02                     | 0.41              |
| 16:1R:56:LYS:NZ    | 16:1R:88:ALA:HA   | 2.35                     | 0.41              |
| 16:1R:103:ARG:HG2  | 16:1R:105:GLY:H   | 1.84                     | 0.41              |
| 18:1T:102:ARG:HD3  | 18:1T:106:ALA:HB1 | 2.01                     | 0.41              |
| 26:11:11:PRO:HG3   | 26:11:30:PRO:HD2  | 2.03                     | 0.41              |
| 35:1a:591:U:H2'    | 35:1a:592:G:C8    | 2.56                     | 0.41              |
| 35:1a:1173:U:H2'   | 35:1a:1174:G:H8   | 1.86                     | 0.41              |
| 38:1d:123:MET:HA   | 38:1d:128:VAL:HA  | 2.02                     | 0.41              |
| 41:1g:137:ARG:HH11 | 41:1g:141:HIS:HE1 | 1.67                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:975:A:H62     | 1:1A:988:A:H2      | 1.69                     | 0.41              |
| 1:1A:1080:A:H1'    | 11:1K:127:SER:HA   | 2.01                     | 0.41              |
| 1:1A:1405:U:H2'    | 1:1A:1406:U:C6     | 2.56                     | 0.41              |
| 1:1A:1808:A:C6     | 26:11:27:ARG:HD2   | 2.56                     | 0.41              |
| 35:1a:393:A:H2'    | 35:1a:394:G:H8     | 1.85                     | 0.41              |
| 35:1a:708:C:H4'    | 45:1k:38:GLY:HA3   | 2.03                     | 0.41              |
| 35:1a:1296:C:H4'   | 35:1a:1302:C:N4    | 2.35                     | 0.41              |
| 35:1a:1493:A:H5'   | 35:1a:1494:G:H5'   | 2.03                     | 0.41              |
| 35:1a:1518:MA6:O2' | 35:1a:1519:MA6:O4' | 2.22                     | 0.41              |
| 38:1d:158:LEU:HD13 | 38:1d:177:MET:HE1  | 2.03                     | 0.41              |
| 40:1f:5:GLU:HB2    | 40:1f:90:MET:HE3   | 2.03                     | 0.41              |
| 54:1t:31:ILE:HG22  | 54:1t:35:TYR:HE2   | 1.85                     | 0.41              |
| 1:1A:825:A:H2'     | 1:1A:826:U:C6      | 2.56                     | 0.41              |
| 1:1A:923:G:H4'     | 25:10:25:GLU:HG3   | 2.01                     | 0.41              |
| 1:1A:1131:G:N2     | 1:1A:1132:U:O4     | 2.45                     | 0.41              |
| 1:1A:1291:C:H2'    | 1:1A:1292:G:C8     | 2.54                     | 0.41              |
| 1:1A:1704:C:H5'    | 35:1a:1429:A:O2'   | 2.21                     | 0.41              |
| 1:1A:2052:A:C2     | 1:1A:2618:G:H1'    | 2.56                     | 0.41              |
| 1:1A:2283:C:C5     | 1:1A:2389:G:H2'    | 2.55                     | 0.41              |
| 1:1A:2623:G:H2'    | 1:1A:2624:G:H8     | 1.86                     | 0.41              |
| 1:1A:2624:G:H2'    | 1:1A:2625:G:C8     | 2.56                     | 0.41              |
| 3:1D:77:VAL:HG13   | 3:1D:91:ALA:HB1    | 2.02                     | 0.41              |
| 16:1R:78:LYS:HE2   | 16:1R:83:LEU:HD21  | 2.01                     | 0.41              |
| 22:1X:23:ALA:HB1   | 22:1X:29:THR:HB    | 2.02                     | 0.41              |
| 29:14:9:TYR:CE2    | 29:14:25:ARG:HD3   | 2.56                     | 0.41              |
| 35:1a:1011:C:H2'   | 35:1a:1012:A:H8    | 1.85                     | 0.41              |
| 44:1j:16:ARG:HA    | 44:1j:19:ASP:OD2   | 2.21                     | 0.41              |
| 56:1v:26:G:C5      | 56:1v:27:C:C4      | 3.09                     | 0.41              |
| 1:1A:179:C:H2'     | 1:1A:180:G:H8      | 1.85                     | 0.41              |
| 1:1A:198:C:H1'     | 1:1A:2434:A:N6     | 2.27                     | 0.41              |
| 1:1A:481:G:H4'     | 1:1A:481:G:OP1     | 2.21                     | 0.41              |
| 1:1A:647:G:N2      | 1:1A:2350:C:O3'    | 2.54                     | 0.41              |
| 1:1A:812:C:H2'     | 1:1A:813:U:H6      | 1.86                     | 0.41              |
| 1:1A:1351:C:H2'    | 1:1A:1352:U:C6     | 2.56                     | 0.41              |
| 1:1A:1530:G:N2     | 1:1A:1542:U:H1'    | 2.36                     | 0.41              |
| 1:1A:2060:A:C6     | 1:1A:2502:G:C2     | 3.09                     | 0.41              |
| 1:1A:2355:G:H1'    | 25:10:32:ILE:HD12  | 2.03                     | 0.41              |
| 1:1A:2365:G:H4'    | 25:10:56:PHE:CZ    | 2.55                     | 0.41              |
| 3:1D:177:SER:O     | 3:1D:270:ARG:HG3   | 2.21                     | 0.41              |
| 4:1E:148:GLN:HB2   | 4:1E:152:PRO:HG2   | 2.03                     | 0.41              |
| 9:1I:121:VAL:HG23  | 9:1I:123:ARG:HG3   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:1K:11:GLN:NE2  | 11:1K:56:VAL:HG12  | 2.36                     | 0.41              |
| 14:1P:118:THR:O   | 14:1P:120:VAL:N    | 2.54                     | 0.41              |
| 15:1Q:30:SER:OG   | 15:1Q:106:ASP:OD1  | 2.24                     | 0.41              |
| 21:1W:84:ARG:HG3  | 21:1W:98:LYS:HE3   | 2.02                     | 0.41              |
| 35:1a:797:C:OP1   | 45:1k:125:LYS:HB2  | 2.21                     | 0.41              |
| 35:1a:834:U:H2'   | 35:1a:835:U:C6     | 2.56                     | 0.41              |
| 35:1a:968:A:N7    | 35:1a:1062:U:O2'   | 2.52                     | 0.41              |
| 35:1a:1010:U:H2'  | 35:1a:1011:C:C6    | 2.56                     | 0.41              |
| 35:1a:1301:U:O2'  | 35:1a:1302:C:OP1   | 2.35                     | 0.41              |
| 35:1a:1367:C:OP1  | 43:1i:116:GLY:N    | 2.54                     | 0.41              |
| 35:1a:1376:U:O3'  | 41:1g:94:ARG:NH1   | 2.53                     | 0.41              |
| 35:1a:1475:G:H2'  | 35:1a:1476:A:C8    | 2.56                     | 0.41              |
| 38:1d:113:ALA:O   | 38:1d:117:VAL:HG23 | 2.20                     | 0.41              |
| 39:1e:80:LEU:HG   | 39:1e:146:MET:SD   | 2.60                     | 0.41              |
| 41:1g:69:ARG:HA   | 41:1g:99:ALA:HB2   | 2.03                     | 0.41              |
| 44:1j:26:VAL:HG13 | 44:1j:36:VAL:HG21  | 2.03                     | 0.41              |
| 45:1k:43:TRP:CZ3  | 45:1k:45:THR:HG23  | 2.55                     | 0.41              |
| 55:1u:25:ALA:O    | 55:1u:29:ALA:HB3   | 2.21                     | 0.41              |
| 1:1A:2068:U:H6    | 1:1A:2068:U:H5''   | 1.86                     | 0.41              |
| 1:1A:2137:U:H2'   | 1:1A:2138:G:H8     | 1.86                     | 0.41              |
| 7:1H:136:ASP:OD2  | 7:1H:138:GLN:HB3   | 2.21                     | 0.41              |
| 11:1K:80:LYS:O    | 11:1K:84:GLY:N     | 2.54                     | 0.41              |
| 35:1a:62:U:H2'    | 35:1a:63:C:C6      | 2.56                     | 0.41              |
| 35:1a:88:U:H2'    | 35:1a:89:U:C6      | 2.56                     | 0.41              |
| 35:1a:418:C:H2'   | 35:1a:419:C:C6     | 2.56                     | 0.41              |
| 35:1a:676:A:C6    | 35:1a:677:U:C4     | 3.09                     | 0.41              |
| 35:1a:790:A:OP1   | 58:1x:38:A:O2'     | 2.38                     | 0.41              |
| 35:1a:831:A:H5'   | 36:1b:20:ARG:HD2   | 2.03                     | 0.41              |
| 54:1t:23:ARG:NH2  | 54:1t:60:GLN:HE22  | 2.19                     | 0.41              |
| 1:1A:1:G:H1       | 1:1A:2902:C:N4     | 2.17                     | 0.40              |
| 1:1A:562:U:H2'    | 1:1A:572:A:O4'     | 2.21                     | 0.40              |
| 1:1A:720:U:H2'    | 1:1A:721:A:H8      | 1.85                     | 0.40              |
| 1:1A:759:G:H2'    | 1:1A:760:G:H8      | 1.86                     | 0.40              |
| 1:1A:817:C:H42    | 1:1A:1190:G:H1     | 1.69                     | 0.40              |
| 1:1A:1429:G:H2'   | 1:1A:1430:G:C8     | 2.56                     | 0.40              |
| 1:1A:1689:A:H2'   | 1:1A:1690:A:C8     | 2.56                     | 0.40              |
| 1:1A:1915:3TD:H3' | 1:1A:1916:A:H8     | 1.86                     | 0.40              |
| 3:1D:52:HIS:CE1   | 3:1D:218:THR:HA    | 2.56                     | 0.40              |
| 16:1R:79:LEU:O    | 16:1R:81:ASN:N     | 2.49                     | 0.40              |
| 18:1T:47:ILE:HB   | 18:1T:96:LEU:HB2   | 2.03                     | 0.40              |
| 22:1X:15:HIS:HE1  | 22:1X:17:SER:HB3   | 1.85                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:1Z:72:VAL:HB   | 24:1Z:91:PHE:HB3  | 2.03                     | 0.40              |
| 35:1a:24:U:H2'    | 35:1a:25:C:C6     | 2.57                     | 0.40              |
| 35:1a:117:G:O6    | 35:1a:289:G:H1'   | 2.21                     | 0.40              |
| 35:1a:1143:G:H2'  | 35:1a:1144:G:H8   | 1.84                     | 0.40              |
| 1:1A:110:G:H2'    | 1:1A:111:A:C8     | 2.56                     | 0.40              |
| 1:1A:182:A:H2'    | 1:1A:183:C:C6     | 2.55                     | 0.40              |
| 1:1A:372:G:H4'    | 1:1A:373:U:H5'    | 2.03                     | 0.40              |
| 1:1A:558:U:OP2    | 12:1N:113:PRO:HD2 | 2.22                     | 0.40              |
| 1:1A:729:G:H2'    | 1:1A:1775:U:H1'   | 2.03                     | 0.40              |
| 1:1A:827:U:OP2    | 1:1A:828:U:N3     | 2.55                     | 0.40              |
| 1:1A:1132:U:H2'   | 1:1A:1133:A:C8    | 2.57                     | 0.40              |
| 1:1A:1448:G:H2'   | 1:1A:1449:G:C8    | 2.56                     | 0.40              |
| 1:1A:1827:U:OP1   | 1:1A:1971:U:H4'   | 2.21                     | 0.40              |
| 1:1A:1958:C:H2'   | 1:1A:1959:G:H8    | 1.86                     | 0.40              |
| 1:1A:2146:C:H4'   | 1:1A:2147:A:C4    | 2.56                     | 0.40              |
| 1:1A:2333:A:H4'   | 1:1A:2334:U:O5'   | 2.21                     | 0.40              |
| 24:1Z:20:LEU:HD11 | 24:1Z:41:GLU:HG3  | 2.03                     | 0.40              |
| 25:10:49:CYS:SG   | 25:10:53:HIS:HA   | 2.60                     | 0.40              |
| 33:18:31:ILE:O    | 33:18:35:LYS:NZ   | 2.44                     | 0.40              |
| 35:1a:71:A:C8     | 35:1a:100:G:C6    | 3.10                     | 0.40              |
| 35:1a:85:U:H5''   | 35:1a:86:G:OP1    | 2.21                     | 0.40              |
| 35:1a:219:U:H2'   | 35:1a:220:G:C8    | 2.56                     | 0.40              |
| 35:1a:398:U:H2'   | 35:1a:399:G:C8    | 2.56                     | 0.40              |
| 35:1a:460:A:H2'   | 35:1a:461:A:C8    | 2.57                     | 0.40              |
| 35:1a:546:A:OP1   | 38:1d:69:ARG:N    | 2.34                     | 0.40              |
| 35:1a:973:G:H1'   | 44:1j:56:HIS:CD2  | 2.56                     | 0.40              |
| 35:1a:1239:A:H4'  | 35:1a:1241:G:C8   | 2.57                     | 0.40              |
| 35:1a:1332:A:H2'  | 35:1a:1333:A:C8   | 2.56                     | 0.40              |
| 35:1a:1525:G:H2'  | 35:1a:1526:G:C8   | 2.56                     | 0.40              |
| 37:1c:63:ILE:HG23 | 37:1c:98:ALA:HA   | 2.03                     | 0.40              |
| 42:1h:9:MET:HG3   | 42:1h:26:MET:SD   | 2.61                     | 0.40              |
| 43:1i:44:ARG:HG3  | 43:1i:48:ARG:NH2  | 2.36                     | 0.40              |
| 1:1A:96:C:H2'     | 1:1A:97:C:C6      | 2.57                     | 0.40              |
| 1:1A:269:C:H2'    | 1:1A:270:A:C8     | 2.50                     | 0.40              |
| 1:1A:323:C:H2'    | 1:1A:1205:A:N1    | 2.37                     | 0.40              |
| 1:1A:481:G:O2'    | 1:1A:506:G:N2     | 2.54                     | 0.40              |
| 1:1A:814:C:H1'    | 1:1A:1225:G:H21   | 1.86                     | 0.40              |
| 1:1A:873:C:H2'    | 1:1A:874:G:H8     | 1.87                     | 0.40              |
| 1:1A:1447:C:O2'   | 1:1A:1544:A:N3    | 2.53                     | 0.40              |
| 1:1A:1614:A:N1    | 21:1W:87:PRO:HA   | 2.36                     | 0.40              |
| 1:1A:1654:A:H2'   | 1:1A:1655:A:C8    | 2.56                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:1874:C:H2'    | 1:1A:1875:G:O4'   | 2.21                     | 0.40              |
| 1:1A:2080:A:OP1    | 26:11:19:HIS:HB3  | 2.21                     | 0.40              |
| 1:1A:2093:G:OP2    | 9:1I:22:LYS:HD3   | 2.21                     | 0.40              |
| 1:1A:2848:G:O2'    | 1:1A:2868:A:N6    | 2.54                     | 0.40              |
| 1:1A:2849:U:OP1    | 18:1T:92:ARG:HB2  | 2.22                     | 0.40              |
| 3:1D:145:MET:HG2   | 3:1D:152:GLN:HG3  | 2.04                     | 0.40              |
| 4:1E:37:VAL:HG23   | 4:1E:92:VAL:HG22  | 2.02                     | 0.40              |
| 12:1N:109:LEU:HD22 | 12:1N:118:MET:SD  | 2.61                     | 0.40              |
| 24:1Z:31:TYR:HB3   | 24:1Z:37:PRO:HB3  | 2.02                     | 0.40              |
| 27:12:26:PHE:HD1   | 27:12:29:ARG:NH1  | 2.20                     | 0.40              |
| 35:1a:376:G:H2'    | 35:1a:377:G:H8    | 1.86                     | 0.40              |
| 35:1a:659:U:OP1    | 49:1o:4:THR:HG23  | 2.21                     | 0.40              |
| 35:1a:770:C:H2'    | 35:1a:771:G:C8    | 2.55                     | 0.40              |
| 35:1a:1498:UR3:H1' | 35:1a:1499:A:N7   | 2.37                     | 0.40              |
| 35:1a:1522:U:H2'   | 35:1a:1523:G:C8   | 2.56                     | 0.40              |
| 42:1h:85:TYR:CD1   | 42:1h:123:GLU:HB2 | 2.56                     | 0.40              |
| 46:1l:33:CYS:HB2   | 46:1l:79:ILE:HG12 | 2.03                     | 0.40              |
| 47:1m:86:ARG:HG3   | 53:1s:72:GLU:OE1  | 2.20                     | 0.40              |
| 1:1A:419:U:H2'     | 1:1A:420:C:C6     | 2.56                     | 0.40              |
| 1:1A:755:U:O4      | 1:1A:756:A:N6     | 2.55                     | 0.40              |
| 1:1A:813:U:C4      | 14:1P:25:SER:HA   | 2.56                     | 0.40              |
| 1:1A:981:A:N1      | 1:1A:2027:G:O2'   | 2.51                     | 0.40              |
| 1:1A:1040:A:H2'    | 1:1A:1041:G:C8    | 2.56                     | 0.40              |
| 1:1A:1289:C:H2'    | 1:1A:1290:C:C6    | 2.56                     | 0.40              |
| 1:1A:2050:C:N4     | 1:1A:2051:A:N1    | 2.69                     | 0.40              |
| 1:1A:2200:C:H2'    | 1:1A:2201:G:C8    | 2.57                     | 0.40              |
| 1:1A:2241:A:H2'    | 1:1A:2242:G:C8    | 2.56                     | 0.40              |
| 1:1A:2399:G:H2'    | 1:1A:2400:G:C8    | 2.57                     | 0.40              |
| 1:1A:2415:G:C6     | 1:1A:2416:C:C4    | 3.09                     | 0.40              |
| 1:1A:2464:G:C2     | 1:1A:2487:G:C2    | 3.10                     | 0.40              |
| 1:1A:2586:U:H2'    | 1:1A:2587:A:C8    | 2.56                     | 0.40              |
| 5:1F:189:THR:O     | 5:1F:193:VAL:HG23 | 2.22                     | 0.40              |
| 6:1G:24:VAL:O      | 6:1G:27:VAL:HG12  | 2.22                     | 0.40              |
| 12:1N:80:HIS:ND1   | 12:1N:81:ILE:HG22 | 2.36                     | 0.40              |
| 17:1S:26:LEU:HD13  | 17:1S:39:VAL:HG22 | 2.04                     | 0.40              |
| 23:1Y:65:GLN:HB2   | 23:1Y:68:ASN:OD1  | 2.21                     | 0.40              |
| 35:1a:17:U:H2'     | 35:1a:18:C:C6     | 2.57                     | 0.40              |
| 35:1a:76:G:N2      | 35:1a:95:C:N3     | 2.69                     | 0.40              |
| 35:1a:898:G:N2     | 35:1a:900:A:H3'   | 2.37                     | 0.40              |
| 35:1a:976:G:H2'    | 35:1a:1362:A:N1   | 2.36                     | 0.40              |
| 35:1a:1420:U:H2'   | 35:1a:1421:G:H8   | 1.87                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:1f:51:ILE:CG2  | 40:1f:86:ARG:HH12 | 2.35                     | 0.40              |
| 41:1g:25:PHE:HD1  | 41:1g:100:MET:HB3 | 1.86                     | 0.40              |
| 46:1l:73:LEU:HD11 | 46:1l:103:CYS:SG  | 2.62                     | 0.40              |
| 48:1n:36:ALA:C    | 48:1n:38:ASP:H    | 2.30                     | 0.40              |
| 51:1q:22:VAL:HG11 | 51:1q:60:ILE:HD11 | 2.03                     | 0.40              |
| 58:1x:29:C:H2'    | 58:1x:30:C:C6     | 2.56                     | 0.40              |
| 1:1A:6:A:H2'      | 1:1A:7:G:C8       | 2.56                     | 0.40              |
| 1:1A:19:A:H5''    | 19:1U:21:LYS:HG2  | 2.02                     | 0.40              |
| 1:1A:227:A:H1'    | 1:1A:229:C:C4     | 2.56                     | 0.40              |
| 1:1A:894:U:H2'    | 1:1A:895:U:O4'    | 2.22                     | 0.40              |
| 1:1A:1165:A:H2'   | 1:1A:1166:G:C8    | 2.56                     | 0.40              |
| 1:1A:1363:C:C2    | 1:1A:1364:G:C8    | 3.09                     | 0.40              |
| 1:1A:1837:C:H2'   | 1:1A:1899:A:H61   | 1.85                     | 0.40              |
| 1:1A:2720:U:OP1   | 18:1T:52:ARG:NH2  | 2.52                     | 0.40              |
| 6:1G:176:PHE:HD1  | 6:1G:176:PHE:HA   | 1.77                     | 0.40              |
| 25:10:45:ALA:O    | 25:10:47:VAL:HG23 | 2.22                     | 0.40              |
| 29:14:33:ASN:OD1  | 29:14:34:LEU:N    | 2.54                     | 0.40              |
| 30:15:12:ARG:HG3  | 30:15:15:ARG:NH1  | 2.36                     | 0.40              |
| 35:1a:1316:G:H4'  | 48:1n:58:SER:OG   | 2.21                     | 0.40              |
| 36:1b:23:ASN:ND2  | 36:1b:190:SER:O   | 2.55                     | 0.40              |
| 37:1c:184:ASN:OD1 | 37:1c:185:THR:N   | 2.54                     | 0.40              |
| 40:1f:76:THR:HB   | 40:1f:80:PHE:CE2  | 2.57                     | 0.40              |
| 55:1u:20:ARG:HB3  | 55:1u:24:LYS:HD2  | 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  |
|-----|-------|---------------|-----------|---------|----------|--------------|
| 3   | 1D    | 269/273 (98%) | 242 (90%) | 23 (9%) | 4 (2%)   | <b>8</b> 37  |
| 4   | 1E    | 207/209 (99%) | 187 (90%) | 19 (9%) | 1 (0%)   | 24 <b>59</b> |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 5   | 1F    | 199/201 (99%) | 185 (93%) | 11 (6%)  | 3 (2%)   | 8           | 37  |
| 6   | 1G    | 175/179 (98%) | 153 (87%) | 19 (11%) | 3 (2%)   | 7           | 35  |
| 7   | 1H    | 174/177 (98%) | 154 (88%) | 18 (10%) | 2 (1%)   | 11          | 43  |
| 8   | 1L    | 67/121 (55%)  | 64 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 9   | 1I    | 147/149 (99%) | 130 (88%) | 13 (9%)  | 4 (3%)   | 4           | 28  |
| 10  | 1J    | 129/165 (78%) | 101 (78%) | 23 (18%) | 5 (4%)   | 2           | 21  |
| 11  | 1K    | 139/142 (98%) | 118 (85%) | 14 (10%) | 7 (5%)   | 1           | 18  |
| 12  | 1N    | 140/142 (99%) | 132 (94%) | 6 (4%)   | 2 (1%)   | 9           | 38  |
| 13  | 1O    | 120/123 (98%) | 106 (88%) | 11 (9%)  | 3 (2%)   | 4           | 29  |
| 14  | 1P    | 141/144 (98%) | 120 (85%) | 16 (11%) | 5 (4%)   | 3           | 23  |
| 15  | 1Q    | 134/136 (98%) | 120 (90%) | 9 (7%)   | 5 (4%)   | 2           | 22  |
| 16  | 1R    | 118/127 (93%) | 103 (87%) | 13 (11%) | 2 (2%)   | 7           | 35  |
| 17  | 1S    | 114/117 (97%) | 103 (90%) | 9 (8%)   | 2 (2%)   | 6           | 34  |
| 18  | 1T    | 112/115 (97%) | 105 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 19  | 1U    | 115/118 (98%) | 113 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 20  | 1V    | 101/103 (98%) | 89 (88%)  | 8 (8%)   | 4 (4%)   | 2           | 21  |
| 21  | 1W    | 108/110 (98%) | 96 (89%)  | 12 (11%) | 0        | 100         | 100 |
| 22  | 1X    | 91/100 (91%)  | 80 (88%)  | 9 (10%)  | 2 (2%)   | 5           | 31  |
| 23  | 1Y    | 100/104 (96%) | 86 (86%)  | 12 (12%) | 2 (2%)   | 6           | 32  |
| 24  | 1Z    | 92/94 (98%)   | 87 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 25  | 10    | 73/85 (86%)   | 68 (93%)  | 5 (7%)   | 0        | 100         | 100 |
| 26  | 11    | 75/78 (96%)   | 71 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 27  | 12    | 61/63 (97%)   | 59 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 28  | 13    | 56/59 (95%)   | 53 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 29  | 14    | 64/70 (91%)   | 53 (83%)  | 10 (16%) | 1 (2%)   | 7           | 36  |
| 30  | 15    | 54/57 (95%)   | 51 (94%)  | 2 (4%)   | 1 (2%)   | 6           | 33  |
| 31  | 16    | 48/55 (87%)   | 42 (88%)  | 5 (10%)  | 1 (2%)   | 5           | 31  |
| 32  | 17    | 44/46 (96%)   | 42 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 33  | 18    | 62/65 (95%)   | 58 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 34  | 19    | 36/38 (95%)   | 30 (83%)  | 5 (14%)  | 1 (3%)   | 4           | 27  |
| 36  | 1b    | 216/241 (90%) | 187 (87%) | 24 (11%) | 5 (2%)   | 5           | 30  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 37  | 1c    | 204/233 (88%)   | 190 (93%)  | 12 (6%)  | 2 (1%)   | 12          | 45  |
| 38  | 1d    | 203/206 (98%)   | 179 (88%)  | 20 (10%) | 4 (2%)   | 6           | 32  |
| 39  | 1e    | 155/167 (93%)   | 136 (88%)  | 11 (7%)  | 8 (5%)   | 1           | 17  |
| 40  | 1f    | 98/135 (73%)    | 87 (89%)   | 6 (6%)   | 5 (5%)   | 1           | 17  |
| 41  | 1g    | 149/179 (83%)   | 129 (87%)  | 15 (10%) | 5 (3%)   | 3           | 24  |
| 42  | 1h    | 127/130 (98%)   | 115 (91%)  | 11 (9%)  | 1 (1%)   | 16          | 50  |
| 43  | 1i    | 125/130 (96%)   | 107 (86%)  | 12 (10%) | 6 (5%)   | 2           | 18  |
| 44  | 1j    | 96/103 (93%)    | 80 (83%)   | 10 (10%) | 6 (6%)   | 1           | 15  |
| 45  | 1k    | 114/129 (88%)   | 98 (86%)   | 14 (12%) | 2 (2%)   | 6           | 34  |
| 46  | 1l    | 121/124 (98%)   | 100 (83%)  | 14 (12%) | 7 (6%)   | 1           | 16  |
| 47  | 1m    | 112/118 (95%)   | 102 (91%)  | 7 (6%)   | 3 (3%)   | 4           | 28  |
| 48  | 1n    | 98/101 (97%)    | 83 (85%)   | 9 (9%)   | 6 (6%)   | 1           | 15  |
| 49  | 1o    | 86/89 (97%)     | 76 (88%)   | 6 (7%)   | 4 (5%)   | 2           | 19  |
| 50  | 1p    | 80/82 (98%)     | 70 (88%)   | 9 (11%)  | 1 (1%)   | 9           | 40  |
| 51  | 1q    | 78/84 (93%)     | 65 (83%)   | 10 (13%) | 3 (4%)   | 2           | 21  |
| 52  | 1r    | 63/75 (84%)     | 57 (90%)   | 3 (5%)   | 3 (5%)   | 2           | 18  |
| 53  | 1s    | 77/92 (84%)     | 70 (91%)   | 6 (8%)   | 1 (1%)   | 9           | 40  |
| 54  | 1t    | 83/87 (95%)     | 78 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 55  | 1u    | 63/71 (89%)     | 45 (71%)   | 11 (18%) | 7 (11%)  | 0           | 6   |
| 57  | 1w    | 637/639 (100%)  | 548 (86%)  | 58 (9%)  | 31 (5%)  | 1           | 18  |
| All | All   | 6550/6980 (94%) | 5803 (89%) | 577 (9%) | 170 (3%) | 6           | 28  |

All (170) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 1G    | 18  | GLU  |
| 7   | 1H    | 108 | PHE  |
| 11  | 1K    | 22  | PRO  |
| 11  | 1K    | 92  | PRO  |
| 12  | 1N    | 81  | ILE  |
| 14  | 1P    | 85  | VAL  |
| 15  | 1Q    | 6   | ARG  |
| 20  | 1V    | 55  | ASP  |
| 37  | 1c    | 96  | VAL  |
| 37  | 1c    | 156 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | 1e    | 122 | VAL  |
| 40  | 1f    | 92  | THR  |
| 41  | 1g    | 16  | LYS  |
| 43  | 1i    | 90  | ASP  |
| 52  | 1r    | 17  | VAL  |
| 57  | 1w    | 8   | VAL  |
| 57  | 1w    | 76  | PRO  |
| 57  | 1w    | 96  | ILE  |
| 57  | 1w    | 176 | ASP  |
| 57  | 1w    | 334 | PRO  |
| 57  | 1w    | 342 | PRO  |
| 57  | 1w    | 344 | PRO  |
| 57  | 1w    | 416 | PRO  |
| 57  | 1w    | 433 | HIS  |
| 57  | 1w    | 438 | PRO  |
| 57  | 1w    | 612 | VAL  |
| 57  | 1w    | 617 | PRO  |
| 57  | 1w    | 624 | PRO  |
| 9   | 1I    | 9   | VAL  |
| 10  | 1J    | 55  | VAL  |
| 10  | 1J    | 90  | GLY  |
| 11  | 1K    | 12  | VAL  |
| 11  | 1K    | 64  | ARG  |
| 12  | 1N    | 82  | GLY  |
| 14  | 1P    | 111 | ILE  |
| 14  | 1P    | 128 | THR  |
| 15  | 1Q    | 10  | ARG  |
| 15  | 1Q    | 23  | GLY  |
| 20  | 1V    | 43  | ASN  |
| 22  | 1X    | 71  | GLY  |
| 23  | 1Y    | 6   | ARG  |
| 38  | 1d    | 26  | ALA  |
| 38  | 1d    | 152 | SER  |
| 41  | 1g    | 29  | LEU  |
| 41  | 1g    | 145 | GLU  |
| 42  | 1h    | 74  | ILE  |
| 43  | 1i    | 57  | VAL  |
| 43  | 1i    | 120 | ALA  |
| 44  | 1j    | 57  | VAL  |
| 45  | 1k    | 88  | PRO  |
| 46  | 1l    | 33  | CYS  |
| 47  | 1m    | 6   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | 1n    | 35  | ASN  |
| 48  | 1n    | 54  | ASP  |
| 55  | 1u    | 12  | ASP  |
| 55  | 1u    | 32  | ARG  |
| 57  | 1w    | 80  | ASP  |
| 3   | 1D    | 204 | LEU  |
| 11  | 1K    | 20  | SER  |
| 14  | 1P    | 94  | THR  |
| 16  | 1R    | 59  | SER  |
| 16  | 1R    | 117 | ASP  |
| 17  | 1S    | 66  | GLY  |
| 23  | 1Y    | 97  | SER  |
| 36  | 1b    | 71  | THR  |
| 41  | 1g    | 56  | SER  |
| 41  | 1g    | 64  | ALA  |
| 43  | 1i    | 13  | SER  |
| 43  | 1i    | 125 | GLN  |
| 44  | 1j    | 35  | GLN  |
| 44  | 1j    | 75  | ASP  |
| 45  | 1k    | 92  | ARG  |
| 46  | 1l    | 23  | LEU  |
| 46  | 1l    | 76  | HIS  |
| 47  | 1m    | 113 | LYS  |
| 48  | 1n    | 3   | LYS  |
| 48  | 1n    | 38  | ASP  |
| 49  | 1o    | 2   | LEU  |
| 49  | 1o    | 45  | HIS  |
| 51  | 1q    | 49  | ASN  |
| 52  | 1r    | 18  | GLN  |
| 55  | 1u    | 30  | GLU  |
| 55  | 1u    | 37  | TYR  |
| 57  | 1w    | 40  | THR  |
| 57  | 1w    | 262 | ARG  |
| 3   | 1D    | 231 | HIS  |
| 5   | 1F    | 83  | VAL  |
| 5   | 1F    | 122 | GLU  |
| 6   | 1G    | 176 | PHE  |
| 9   | 1I    | 41  | LYS  |
| 10  | 1J    | 22  | ALA  |
| 10  | 1J    | 88  | HIS  |
| 11  | 1K    | 100 | ILE  |
| 13  | 1O    | 109 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | 1O    | 110 | GLU  |
| 14  | 1P    | 29  | LYS  |
| 17  | 1S    | 100 | HIS  |
| 22  | 1X    | 37  | ASP  |
| 29  | 14    | 26  | SER  |
| 31  | 16    | 45  | HIS  |
| 34  | 19    | 29  | ALA  |
| 36  | 1b    | 11  | ALA  |
| 36  | 1b    | 126 | ASP  |
| 38  | 1d    | 166 | LYS  |
| 38  | 1d    | 191 | SER  |
| 39  | 1e    | 53  | ARG  |
| 39  | 1e    | 98  | ALA  |
| 40  | 1f    | 54  | LEU  |
| 40  | 1f    | 56  | LYS  |
| 40  | 1f    | 63  | ASN  |
| 40  | 1f    | 86  | ARG  |
| 44  | 1j    | 29  | ALA  |
| 46  | 1l    | 2   | THR  |
| 46  | 1l    | 35  | ARG  |
| 49  | 1o    | 13  | GLU  |
| 50  | 1p    | 8   | ARG  |
| 53  | 1s    | 4   | LEU  |
| 55  | 1u    | 34  | ARG  |
| 55  | 1u    | 65  | ARG  |
| 57  | 1w    | 45  | ASN  |
| 57  | 1w    | 173 | GLU  |
| 57  | 1w    | 244 | ARG  |
| 57  | 1w    | 289 | ILE  |
| 57  | 1w    | 354 | LYS  |
| 57  | 1w    | 414 | THR  |
| 57  | 1w    | 609 | GLY  |
| 4   | 1E    | 149 | ASN  |
| 5   | 1F    | 149 | ILE  |
| 7   | 1H    | 45  | ALA  |
| 9   | 1I    | 3   | VAL  |
| 9   | 1I    | 15  | LEU  |
| 10  | 1J    | 118 | ILE  |
| 15  | 1Q    | 70  | ASP  |
| 20  | 1V    | 53  | PHE  |
| 30  | 15    | 2   | VAL  |
| 36  | 1b    | 19  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | 1e    | 23  | THR  |
| 39  | 1e    | 77  | ASN  |
| 39  | 1e    | 121 | ASN  |
| 44  | 1j    | 33  | GLY  |
| 46  | 1l    | 42  | LYS  |
| 46  | 1l    | 88  | ASP  |
| 48  | 1n    | 23  | LYS  |
| 48  | 1n    | 100 | SER  |
| 49  | 1o    | 87  | ARG  |
| 51  | 1q    | 17  | GLU  |
| 52  | 1r    | 46  | THR  |
| 57  | 1w    | 350 | VAL  |
| 57  | 1w    | 371 | SER  |
| 57  | 1w    | 419 | ILE  |
| 57  | 1w    | 613 | THR  |
| 11  | 1K    | 3   | LYS  |
| 20  | 1V    | 54  | VAL  |
| 36  | 1b    | 87  | ASP  |
| 39  | 1e    | 102 | THR  |
| 43  | 1i    | 9   | GLY  |
| 57  | 1w    | 41  | THR  |
| 15  | 1Q    | 69  | PRO  |
| 51  | 1q    | 20  | ILE  |
| 57  | 1w    | 75  | THR  |
| 3   | 1D    | 236 | GLY  |
| 3   | 1D    | 253 | GLY  |
| 39  | 1e    | 93  | VAL  |
| 44  | 1j    | 41  | PRO  |
| 57  | 1w    | 621 | PRO  |
| 13  | 1O    | 35  | VAL  |
| 47  | 1m    | 9   | PRO  |
| 6   | 1G    | 175 | PRO  |
| 55  | 1u    | 9   | GLU  |
| 57  | 1w    | 387 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3   | 1D    | 216/218 (99%)  | 216 (100%) | 0        | 100         | 100 |
| 4   | 1E    | 164/164 (100%) | 164 (100%) | 0        | 100         | 100 |
| 5   | 1F    | 165/165 (100%) | 164 (99%)  | 1 (1%)   | 78          | 80  |
| 6   | 1G    | 148/150 (99%)  | 148 (100%) | 0        | 100         | 100 |
| 7   | 1H    | 137/138 (99%)  | 137 (100%) | 0        | 100         | 100 |
| 9   | 1I    | 114/114 (100%) | 114 (100%) | 0        | 100         | 100 |
| 10  | 1J    | 100/123 (81%)  | 100 (100%) | 0        | 100         | 100 |
| 11  | 1K    | 109/110 (99%)  | 109 (100%) | 0        | 100         | 100 |
| 12  | 1N    | 116/116 (100%) | 116 (100%) | 0        | 100         | 100 |
| 13  | 1O    | 103/104 (99%)  | 101 (98%)  | 2 (2%)   | 50          | 66  |
| 14  | 1P    | 102/103 (99%)  | 102 (100%) | 0        | 100         | 100 |
| 15  | 1Q    | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 16  | 1R    | 100/103 (97%)  | 100 (100%) | 0        | 100         | 100 |
| 17  | 1S    | 86/87 (99%)    | 86 (100%)  | 0        | 100         | 100 |
| 18  | 1T    | 99/100 (99%)   | 98 (99%)   | 1 (1%)   | 68          | 75  |
| 19  | 1U    | 89/90 (99%)    | 89 (100%)  | 0        | 100         | 100 |
| 20  | 1V    | 84/84 (100%)   | 84 (100%)  | 0        | 100         | 100 |
| 21  | 1W    | 93/93 (100%)   | 92 (99%)   | 1 (1%)   | 65          | 74  |
| 22  | 1X    | 80/84 (95%)    | 80 (100%)  | 0        | 100         | 100 |
| 23  | 1Y    | 83/85 (98%)    | 83 (100%)  | 0        | 100         | 100 |
| 24  | 1Z    | 78/78 (100%)   | 78 (100%)  | 0        | 100         | 100 |
| 25  | 10    | 57/63 (90%)    | 57 (100%)  | 0        | 100         | 100 |
| 26  | 11    | 67/68 (98%)    | 67 (100%)  | 0        | 100         | 100 |
| 27  | 12    | 55/55 (100%)   | 55 (100%)  | 0        | 100         | 100 |
| 28  | 13    | 48/49 (98%)    | 48 (100%)  | 0        | 100         | 100 |
| 29  | 14    | 59/62 (95%)    | 59 (100%)  | 0        | 100         | 100 |
| 30  | 15    | 47/48 (98%)    | 47 (100%)  | 0        | 100         | 100 |
| 31  | 16    | 45/49 (92%)    | 45 (100%)  | 0        | 100         | 100 |
| 32  | 17    | 38/38 (100%)   | 38 (100%)  | 0        | 100         | 100 |
| 33  | 18    | 51/52 (98%)    | 50 (98%)   | 1 (2%)   | 48          | 65  |
| 34  | 19    | 34/34 (100%)   | 34 (100%)  | 0        | 100         | 100 |
| 36  | 1b    | 180/199 (90%)  | 180 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 37  | 1c    | 170/190 (90%)   | 169 (99%)   | 1 (1%)   | 78          | 80  |
| 38  | 1d    | 172/173 (99%)   | 172 (100%)  | 0        | 100         | 100 |
| 39  | 1e    | 114/126 (90%)   | 114 (100%)  | 0        | 100         | 100 |
| 40  | 1f    | 87/116 (75%)    | 87 (100%)   | 0        | 100         | 100 |
| 41  | 1g    | 124/147 (84%)   | 124 (100%)  | 0        | 100         | 100 |
| 42  | 1h    | 104/105 (99%)   | 104 (100%)  | 0        | 100         | 100 |
| 43  | 1i    | 105/107 (98%)   | 105 (100%)  | 0        | 100         | 100 |
| 44  | 1j    | 86/90 (96%)     | 86 (100%)   | 0        | 100         | 100 |
| 45  | 1k    | 89/99 (90%)     | 89 (100%)   | 0        | 100         | 100 |
| 46  | 1l    | 103/104 (99%)   | 103 (100%)  | 0        | 100         | 100 |
| 47  | 1m    | 92/96 (96%)     | 92 (100%)   | 0        | 100         | 100 |
| 48  | 1n    | 79/84 (94%)     | 77 (98%)    | 2 (2%)   | 42          | 62  |
| 49  | 1o    | 76/77 (99%)     | 76 (100%)   | 0        | 100         | 100 |
| 50  | 1p    | 65/65 (100%)    | 65 (100%)   | 0        | 100         | 100 |
| 51  | 1q    | 74/78 (95%)     | 74 (100%)   | 0        | 100         | 100 |
| 52  | 1r    | 48/65 (74%)     | 48 (100%)   | 0        | 100         | 100 |
| 53  | 1s    | 70/79 (89%)     | 70 (100%)   | 0        | 100         | 100 |
| 54  | 1t    | 65/66 (98%)     | 65 (100%)   | 0        | 100         | 100 |
| 55  | 1u    | 44/61 (72%)     | 44 (100%)   | 0        | 100         | 100 |
| 57  | 1w    | 6/576 (1%)      | 6 (100%)    | 0        | 100         | 100 |
| All | All   | 4829/5639 (86%) | 4820 (100%) | 9 (0%)   | 85          | 87  |

All (9) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 1F    | 187 | VAL  |
| 13  | 1O    | 41  | ILE  |
| 13  | 1O    | 58  | LEU  |
| 18  | 1T    | 47  | ILE  |
| 21  | 1W    | 88  | ARG  |
| 33  | 18    | 61  | LEU  |
| 37  | 1c    | 156 | LEU  |
| 48  | 1n    | 34  | VAL  |
| 48  | 1n    | 35  | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1D    | 36  | ASN  |
| 3   | 1D    | 45  | ASN  |
| 3   | 1D    | 85  | ASN  |
| 3   | 1D    | 152 | GLN  |
| 3   | 1D    | 250 | GLN  |
| 4   | 1E    | 32  | ASN  |
| 4   | 1E    | 150 | GLN  |
| 4   | 1E    | 164 | GLN  |
| 4   | 1E    | 173 | GLN  |
| 5   | 1F    | 41  | GLN  |
| 5   | 1F    | 136 | GLN  |
| 5   | 1F    | 156 | ASN  |
| 5   | 1F    | 195 | GLN  |
| 6   | 1G    | 4   | HIS  |
| 7   | 1H    | 72  | ASN  |
| 7   | 1H    | 103 | ASN  |
| 7   | 1H    | 115 | GLN  |
| 7   | 1H    | 138 | GLN  |
| 9   | 1I    | 33  | GLN  |
| 10  | 1J    | 4   | ASN  |
| 10  | 1J    | 9   | GLN  |
| 10  | 1J    | 88  | HIS  |
| 12  | 1N    | 40  | HIS  |
| 12  | 1N    | 58  | ASN  |
| 13  | 1O    | 3   | GLN  |
| 14  | 1P    | 35  | HIS  |
| 15  | 1Q    | 13  | HIS  |
| 15  | 1Q    | 45  | GLN  |
| 16  | 1R    | 9   | GLN  |
| 18  | 1T    | 2   | ASN  |
| 18  | 1T    | 11  | GLN  |
| 20  | 1V    | 86  | GLN  |
| 20  | 1V    | 91  | GLN  |
| 21  | 1W    | 7   | HIS  |
| 21  | 1W    | 61  | ASN  |
| 23  | 1Y    | 68  | ASN  |
| 23  | 1Y    | 73  | ASN  |
| 24  | 1Z    | 87  | GLN  |
| 25  | 10    | 42  | HIS  |
| 26  | 11    | 16  | ASN  |
| 27  | 12    | 25  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | 12    | 27  | ASN  |
| 31  | 16    | 18  | HIS  |
| 34  | 19    | 13  | ASN  |
| 36  | 1b    | 18  | GLN  |
| 36  | 1b    | 41  | ASN  |
| 36  | 1b    | 177 | ASN  |
| 37  | 1c    | 68  | HIS  |
| 37  | 1c    | 138 | GLN  |
| 38  | 1d    | 35  | GLN  |
| 38  | 1d    | 125 | ASN  |
| 38  | 1d    | 151 | GLN  |
| 38  | 1d    | 197 | HIS  |
| 39  | 1e    | 72  | ASN  |
| 40  | 1f    | 11  | HIS  |
| 40  | 1f    | 37  | HIS  |
| 40  | 1f    | 58  | HIS  |
| 41  | 1g    | 141 | HIS  |
| 41  | 1g    | 147 | ASN  |
| 42  | 1h    | 3   | GLN  |
| 42  | 1h    | 66  | GLN  |
| 43  | 1i    | 30  | ASN  |
| 46  | 1l    | 76  | HIS  |
| 48  | 1n    | 60  | GLN  |
| 49  | 1o    | 39  | GLN  |
| 49  | 1o    | 45  | HIS  |
| 49  | 1o    | 61  | GLN  |
| 50  | 1p    | 18  | GLN  |
| 50  | 1p    | 79  | ASN  |
| 51  | 1q    | 8   | GLN  |
| 51  | 1q    | 30  | HIS  |
| 51  | 1q    | 44  | HIS  |
| 53  | 1s    | 13  | HIS  |
| 53  | 1s    | 51  | HIS  |
| 53  | 1s    | 56  | HIS  |
| 53  | 1s    | 68  | HIS  |
| 54  | 1t    | 2   | ASN  |
| 54  | 1t    | 60  | GLN  |
| 54  | 1t    | 81  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1A    | 2898/2904 (99%) | 427 (14%)         | 33 (1%)         |
| 2   | 1B    | 119/120 (99%)   | 14 (11%)          | 2 (1%)          |
| 35  | 1a    | 1538/1539 (99%) | 181 (11%)         | 0               |
| 56  | 1v    | 8/60 (13%)      | 0                 | 0               |
| 58  | 1x    | 70/77 (90%)     | 5 (7%)            | 0               |
| All | All   | 4633/4700 (98%) | 627 (13%)         | 35 (0%)         |

All (627) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 10  | A    |
| 1   | 1A    | 12  | U    |
| 1   | 1A    | 27  | G    |
| 1   | 1A    | 34  | U    |
| 1   | 1A    | 35  | G    |
| 1   | 1A    | 42  | A    |
| 1   | 1A    | 46  | G    |
| 1   | 1A    | 49  | A    |
| 1   | 1A    | 51  | G    |
| 1   | 1A    | 52  | A    |
| 1   | 1A    | 71  | A    |
| 1   | 1A    | 74  | A    |
| 1   | 1A    | 75  | G    |
| 1   | 1A    | 84  | A    |
| 1   | 1A    | 91  | A    |
| 1   | 1A    | 92  | U    |
| 1   | 1A    | 118 | A    |
| 1   | 1A    | 120 | U    |
| 1   | 1A    | 138 | U    |
| 1   | 1A    | 139 | U    |
| 1   | 1A    | 140 | C    |
| 1   | 1A    | 141 | G    |
| 1   | 1A    | 142 | A    |
| 1   | 1A    | 162 | U    |
| 1   | 1A    | 163 | C    |
| 1   | 1A    | 181 | A    |
| 1   | 1A    | 196 | A    |
| 1   | 1A    | 199 | A    |
| 1   | 1A    | 205 | G    |
| 1   | 1A    | 206 | U    |
| 1   | 1A    | 216 | A    |
| 1   | 1A    | 221 | A    |
| 1   | 1A    | 222 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 228 | C    |
| 1   | 1A    | 242 | G    |
| 1   | 1A    | 243 | U    |
| 1   | 1A    | 248 | G    |
| 1   | 1A    | 249 | C    |
| 1   | 1A    | 255 | A    |
| 1   | 1A    | 266 | G    |
| 1   | 1A    | 267 | C    |
| 1   | 1A    | 276 | U    |
| 1   | 1A    | 278 | A    |
| 1   | 1A    | 294 | A    |
| 1   | 1A    | 301 | G    |
| 1   | 1A    | 310 | A    |
| 1   | 1A    | 311 | A    |
| 1   | 1A    | 323 | C    |
| 1   | 1A    | 324 | A    |
| 1   | 1A    | 329 | G    |
| 1   | 1A    | 330 | A    |
| 1   | 1A    | 353 | C    |
| 1   | 1A    | 361 | G    |
| 1   | 1A    | 367 | G    |
| 1   | 1A    | 371 | A    |
| 1   | 1A    | 372 | G    |
| 1   | 1A    | 373 | U    |
| 1   | 1A    | 386 | G    |
| 1   | 1A    | 387 | U    |
| 1   | 1A    | 391 | A    |
| 1   | 1A    | 404 | A    |
| 1   | 1A    | 406 | G    |
| 1   | 1A    | 411 | G    |
| 1   | 1A    | 424 | G    |
| 1   | 1A    | 456 | C    |
| 1   | 1A    | 457 | A    |
| 1   | 1A    | 458 | G    |
| 1   | 1A    | 459 | U    |
| 1   | 1A    | 480 | A    |
| 1   | 1A    | 481 | G    |
| 1   | 1A    | 491 | G    |
| 1   | 1A    | 504 | A    |
| 1   | 1A    | 505 | A    |
| 1   | 1A    | 506 | G    |
| 1   | 1A    | 529 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 530 | G    |
| 1   | 1A    | 532 | A    |
| 1   | 1A    | 542 | C    |
| 1   | 1A    | 543 | G    |
| 1   | 1A    | 545 | U    |
| 1   | 1A    | 547 | A    |
| 1   | 1A    | 550 | C    |
| 1   | 1A    | 563 | A    |
| 1   | 1A    | 572 | A    |
| 1   | 1A    | 573 | U    |
| 1   | 1A    | 575 | A    |
| 1   | 1A    | 603 | A    |
| 1   | 1A    | 616 | A    |
| 1   | 1A    | 627 | A    |
| 1   | 1A    | 637 | A    |
| 1   | 1A    | 646 | U    |
| 1   | 1A    | 654 | A    |
| 1   | 1A    | 669 | G    |
| 1   | 1A    | 670 | A    |
| 1   | 1A    | 677 | A    |
| 1   | 1A    | 686 | U    |
| 1   | 1A    | 687 | C    |
| 1   | 1A    | 695 | G    |
| 1   | 1A    | 726 | G    |
| 1   | 1A    | 730 | A    |
| 1   | 1A    | 746 | PSU  |
| 1   | 1A    | 747 | 5MU  |
| 1   | 1A    | 748 | G    |
| 1   | 1A    | 752 | A    |
| 1   | 1A    | 753 | A    |
| 1   | 1A    | 764 | A    |
| 1   | 1A    | 765 | C    |
| 1   | 1A    | 776 | G    |
| 1   | 1A    | 782 | A    |
| 1   | 1A    | 784 | G    |
| 1   | 1A    | 785 | G    |
| 1   | 1A    | 789 | A    |
| 1   | 1A    | 792 | A    |
| 1   | 1A    | 800 | A    |
| 1   | 1A    | 805 | G    |
| 1   | 1A    | 812 | C    |
| 1   | 1A    | 819 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 822  | G    |
| 1   | 1A    | 827  | U    |
| 1   | 1A    | 828  | U    |
| 1   | 1A    | 830  | G    |
| 1   | 1A    | 831  | G    |
| 1   | 1A    | 845  | A    |
| 1   | 1A    | 846  | U    |
| 1   | 1A    | 847  | U    |
| 1   | 1A    | 858  | G    |
| 1   | 1A    | 859  | G    |
| 1   | 1A    | 860  | U    |
| 1   | 1A    | 878  | A    |
| 1   | 1A    | 896  | A    |
| 1   | 1A    | 897  | C    |
| 1   | 1A    | 907  | G    |
| 1   | 1A    | 910  | A    |
| 1   | 1A    | 932  | U    |
| 1   | 1A    | 941  | A    |
| 1   | 1A    | 946  | C    |
| 1   | 1A    | 961  | C    |
| 1   | 1A    | 974  | G    |
| 1   | 1A    | 983  | A    |
| 1   | 1A    | 985  | C    |
| 1   | 1A    | 995  | C    |
| 1   | 1A    | 996  | A    |
| 1   | 1A    | 1012 | U    |
| 1   | 1A    | 1013 | C    |
| 1   | 1A    | 1021 | A    |
| 1   | 1A    | 1022 | G    |
| 1   | 1A    | 1023 | U    |
| 1   | 1A    | 1033 | U    |
| 1   | 1A    | 1046 | A    |
| 1   | 1A    | 1047 | G    |
| 1   | 1A    | 1053 | C    |
| 1   | 1A    | 1054 | A    |
| 1   | 1A    | 1057 | A    |
| 1   | 1A    | 1060 | U    |
| 1   | 1A    | 1061 | U    |
| 1   | 1A    | 1062 | G    |
| 1   | 1A    | 1064 | C    |
| 1   | 1A    | 1065 | U    |
| 1   | 1A    | 1066 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1068 | G    |
| 1   | 1A    | 1070 | A    |
| 1   | 1A    | 1071 | G    |
| 1   | 1A    | 1075 | C    |
| 1   | 1A    | 1076 | C    |
| 1   | 1A    | 1079 | C    |
| 1   | 1A    | 1084 | A    |
| 1   | 1A    | 1088 | A    |
| 1   | 1A    | 1104 | C    |
| 1   | 1A    | 1111 | A    |
| 1   | 1A    | 1112 | G    |
| 1   | 1A    | 1119 | U    |
| 1   | 1A    | 1130 | U    |
| 1   | 1A    | 1131 | G    |
| 1   | 1A    | 1132 | U    |
| 1   | 1A    | 1133 | A    |
| 1   | 1A    | 1135 | C    |
| 1   | 1A    | 1143 | A    |
| 1   | 1A    | 1174 | U    |
| 1   | 1A    | 1175 | A    |
| 1   | 1A    | 1176 | U    |
| 1   | 1A    | 1177 | G    |
| 1   | 1A    | 1179 | G    |
| 1   | 1A    | 1180 | U    |
| 1   | 1A    | 1206 | G    |
| 1   | 1A    | 1212 | G    |
| 1   | 1A    | 1247 | A    |
| 1   | 1A    | 1248 | G    |
| 1   | 1A    | 1250 | G    |
| 1   | 1A    | 1251 | C    |
| 1   | 1A    | 1253 | A    |
| 1   | 1A    | 1256 | G    |
| 1   | 1A    | 1271 | G    |
| 1   | 1A    | 1272 | A    |
| 1   | 1A    | 1300 | G    |
| 1   | 1A    | 1301 | A    |
| 1   | 1A    | 1314 | C    |
| 1   | 1A    | 1321 | A    |
| 1   | 1A    | 1329 | U    |
| 1   | 1A    | 1332 | G    |
| 1   | 1A    | 1341 | G    |
| 1   | 1A    | 1345 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1365 | A    |
| 1   | 1A    | 1368 | G    |
| 1   | 1A    | 1378 | A    |
| 1   | 1A    | 1379 | U    |
| 1   | 1A    | 1383 | A    |
| 1   | 1A    | 1416 | G    |
| 1   | 1A    | 1419 | A    |
| 1   | 1A    | 1420 | A    |
| 1   | 1A    | 1428 | C    |
| 1   | 1A    | 1454 | C    |
| 1   | 1A    | 1461 | C    |
| 1   | 1A    | 1482 | G    |
| 1   | 1A    | 1490 | A    |
| 1   | 1A    | 1491 | G    |
| 1   | 1A    | 1504 | A    |
| 1   | 1A    | 1515 | A    |
| 1   | 1A    | 1524 | G    |
| 1   | 1A    | 1533 | C    |
| 1   | 1A    | 1535 | A    |
| 1   | 1A    | 1536 | C    |
| 1   | 1A    | 1537 | G    |
| 1   | 1A    | 1555 | G    |
| 1   | 1A    | 1559 | U    |
| 1   | 1A    | 1560 | G    |
| 1   | 1A    | 1565 | C    |
| 1   | 1A    | 1567 | G    |
| 1   | 1A    | 1569 | A    |
| 1   | 1A    | 1581 | G    |
| 1   | 1A    | 1585 | C    |
| 1   | 1A    | 1611 | C    |
| 1   | 1A    | 1634 | A    |
| 1   | 1A    | 1646 | C    |
| 1   | 1A    | 1647 | U    |
| 1   | 1A    | 1648 | U    |
| 1   | 1A    | 1651 | G    |
| 1   | 1A    | 1654 | A    |
| 1   | 1A    | 1664 | A    |
| 1   | 1A    | 1670 | C    |
| 1   | 1A    | 1674 | G    |
| 1   | 1A    | 1694 | C    |
| 1   | 1A    | 1695 | G    |
| 1   | 1A    | 1715 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1729 | U    |
| 1   | 1A    | 1730 | C    |
| 1   | 1A    | 1732 | C    |
| 1   | 1A    | 1738 | G    |
| 1   | 1A    | 1758 | U    |
| 1   | 1A    | 1764 | C    |
| 1   | 1A    | 1773 | A    |
| 1   | 1A    | 1780 | A    |
| 1   | 1A    | 1781 | U    |
| 1   | 1A    | 1784 | A    |
| 1   | 1A    | 1791 | A    |
| 1   | 1A    | 1800 | C    |
| 1   | 1A    | 1801 | A    |
| 1   | 1A    | 1802 | A    |
| 1   | 1A    | 1808 | A    |
| 1   | 1A    | 1816 | C    |
| 1   | 1A    | 1829 | A    |
| 1   | 1A    | 1833 | C    |
| 1   | 1A    | 1834 | U    |
| 1   | 1A    | 1871 | A    |
| 1   | 1A    | 1890 | A    |
| 1   | 1A    | 1896 | G    |
| 1   | 1A    | 1901 | A    |
| 1   | 1A    | 1906 | G    |
| 1   | 1A    | 1913 | A    |
| 1   | 1A    | 1914 | C    |
| 1   | 1A    | 1915 | 3TD  |
| 1   | 1A    | 1929 | G    |
| 1   | 1A    | 1930 | G    |
| 1   | 1A    | 1937 | A    |
| 1   | 1A    | 1938 | A    |
| 1   | 1A    | 1940 | U    |
| 1   | 1A    | 1941 | C    |
| 1   | 1A    | 1944 | U    |
| 1   | 1A    | 1955 | U    |
| 1   | 1A    | 1962 | 5MC  |
| 1   | 1A    | 1963 | U    |
| 1   | 1A    | 1967 | C    |
| 1   | 1A    | 1970 | A    |
| 1   | 1A    | 1971 | U    |
| 1   | 1A    | 1972 | G    |
| 1   | 1A    | 1991 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1993 | U    |
| 1   | 1A    | 1997 | C    |
| 1   | 1A    | 2021 | C    |
| 1   | 1A    | 2022 | U    |
| 1   | 1A    | 2023 | C    |
| 1   | 1A    | 2030 | 6MZ  |
| 1   | 1A    | 2031 | A    |
| 1   | 1A    | 2033 | A    |
| 1   | 1A    | 2043 | C    |
| 1   | 1A    | 2049 | G    |
| 1   | 1A    | 2052 | A    |
| 1   | 1A    | 2055 | C    |
| 1   | 1A    | 2056 | G    |
| 1   | 1A    | 2060 | A    |
| 1   | 1A    | 2061 | G    |
| 1   | 1A    | 2062 | A    |
| 1   | 1A    | 2068 | U    |
| 1   | 1A    | 2069 | G7M  |
| 1   | 1A    | 2070 | A    |
| 1   | 1A    | 2072 | C    |
| 1   | 1A    | 2093 | G    |
| 1   | 1A    | 2095 | A    |
| 1   | 1A    | 2096 | C    |
| 1   | 1A    | 2098 | U    |
| 1   | 1A    | 2110 | G    |
| 1   | 1A    | 2111 | U    |
| 1   | 1A    | 2112 | G    |
| 1   | 1A    | 2113 | U    |
| 1   | 1A    | 2116 | G    |
| 1   | 1A    | 2118 | U    |
| 1   | 1A    | 2119 | A    |
| 1   | 1A    | 2127 | G    |
| 1   | 1A    | 2131 | U    |
| 1   | 1A    | 2132 | U    |
| 1   | 1A    | 2133 | G    |
| 1   | 1A    | 2145 | C    |
| 1   | 1A    | 2162 | G    |
| 1   | 1A    | 2164 | C    |
| 1   | 1A    | 2170 | A    |
| 1   | 1A    | 2172 | U    |
| 1   | 1A    | 2173 | A    |
| 1   | 1A    | 2192 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2198 | A    |
| 1   | 1A    | 2204 | G    |
| 1   | 1A    | 2211 | A    |
| 1   | 1A    | 2213 | U    |
| 1   | 1A    | 2225 | A    |
| 1   | 1A    | 2226 | C    |
| 1   | 1A    | 2238 | G    |
| 1   | 1A    | 2250 | G    |
| 1   | 1A    | 2251 | OMG  |
| 1   | 1A    | 2252 | G    |
| 1   | 1A    | 2278 | A    |
| 1   | 1A    | 2283 | C    |
| 1   | 1A    | 2287 | A    |
| 1   | 1A    | 2305 | U    |
| 1   | 1A    | 2309 | A    |
| 1   | 1A    | 2320 | U    |
| 1   | 1A    | 2327 | A    |
| 1   | 1A    | 2334 | U    |
| 1   | 1A    | 2335 | A    |
| 1   | 1A    | 2350 | C    |
| 1   | 1A    | 2354 | C    |
| 1   | 1A    | 2361 | G    |
| 1   | 1A    | 2383 | G    |
| 1   | 1A    | 2385 | C    |
| 1   | 1A    | 2391 | G    |
| 1   | 1A    | 2392 | A    |
| 1   | 1A    | 2402 | U    |
| 1   | 1A    | 2407 | A    |
| 1   | 1A    | 2423 | U    |
| 1   | 1A    | 2424 | C    |
| 1   | 1A    | 2426 | A    |
| 1   | 1A    | 2428 | G    |
| 1   | 1A    | 2429 | G    |
| 1   | 1A    | 2430 | A    |
| 1   | 1A    | 2431 | U    |
| 1   | 1A    | 2435 | A    |
| 1   | 1A    | 2441 | U    |
| 1   | 1A    | 2445 | 2MG  |
| 1   | 1A    | 2448 | A    |
| 1   | 1A    | 2476 | A    |
| 1   | 1A    | 2484 | G    |
| 1   | 1A    | 2499 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2502 | G    |
| 1   | 1A    | 2503 | 2MA  |
| 1   | 1A    | 2504 | PSU  |
| 1   | 1A    | 2506 | U    |
| 1   | 1A    | 2513 | A    |
| 1   | 1A    | 2518 | A    |
| 1   | 1A    | 2529 | G    |
| 1   | 1A    | 2547 | A    |
| 1   | 1A    | 2552 | OMU  |
| 1   | 1A    | 2553 | G    |
| 1   | 1A    | 2554 | U    |
| 1   | 1A    | 2567 | G    |
| 1   | 1A    | 2572 | A    |
| 1   | 1A    | 2585 | U    |
| 1   | 1A    | 2586 | U    |
| 1   | 1A    | 2602 | A    |
| 1   | 1A    | 2603 | G    |
| 1   | 1A    | 2609 | U    |
| 1   | 1A    | 2613 | U    |
| 1   | 1A    | 2614 | A    |
| 1   | 1A    | 2629 | U    |
| 1   | 1A    | 2636 | C    |
| 1   | 1A    | 2646 | C    |
| 1   | 1A    | 2655 | G    |
| 1   | 1A    | 2656 | U    |
| 1   | 1A    | 2689 | U    |
| 1   | 1A    | 2690 | U    |
| 1   | 1A    | 2712 | C    |
| 1   | 1A    | 2713 | U    |
| 1   | 1A    | 2714 | G    |
| 1   | 1A    | 2718 | G    |
| 1   | 1A    | 2726 | A    |
| 1   | 1A    | 2739 | U    |
| 1   | 1A    | 2744 | G    |
| 1   | 1A    | 2748 | A    |
| 1   | 1A    | 2757 | A    |
| 1   | 1A    | 2764 | A    |
| 1   | 1A    | 2765 | A    |
| 1   | 1A    | 2778 | A    |
| 1   | 1A    | 2779 | U    |
| 1   | 1A    | 2780 | G    |
| 1   | 1A    | 2791 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2794 | C    |
| 1   | 1A    | 2797 | U    |
| 1   | 1A    | 2799 | A    |
| 1   | 1A    | 2800 | A    |
| 1   | 1A    | 2808 | G    |
| 1   | 1A    | 2809 | A    |
| 1   | 1A    | 2818 | U    |
| 1   | 1A    | 2820 | A    |
| 1   | 1A    | 2833 | U    |
| 1   | 1A    | 2849 | U    |
| 1   | 1A    | 2867 | G    |
| 1   | 1A    | 2868 | A    |
| 1   | 1A    | 2872 | A    |
| 1   | 1A    | 2880 | C    |
| 1   | 1A    | 2893 | A    |
| 1   | 1A    | 2894 | G    |
| 2   | 1B    | 4    | C    |
| 2   | 1B    | 13   | G    |
| 2   | 1B    | 24   | G    |
| 2   | 1B    | 35   | C    |
| 2   | 1B    | 44   | G    |
| 2   | 1B    | 45   | A    |
| 2   | 1B    | 53   | A    |
| 2   | 1B    | 67   | G    |
| 2   | 1B    | 88   | C    |
| 2   | 1B    | 89   | U    |
| 2   | 1B    | 90   | C    |
| 2   | 1B    | 91   | C    |
| 2   | 1B    | 108  | A    |
| 2   | 1B    | 109  | A    |
| 35  | 1a    | 9    | G    |
| 35  | 1a    | 22   | G    |
| 35  | 1a    | 32   | A    |
| 35  | 1a    | 39   | G    |
| 35  | 1a    | 51   | A    |
| 35  | 1a    | 71   | A    |
| 35  | 1a    | 86   | G    |
| 35  | 1a    | 87   | C    |
| 35  | 1a    | 121  | U    |
| 35  | 1a    | 130  | A    |
| 35  | 1a    | 177  | G    |
| 35  | 1a    | 183  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | 1a    | 184 | G    |
| 35  | 1a    | 209 | U    |
| 35  | 1a    | 210 | C    |
| 35  | 1a    | 212 | G    |
| 35  | 1a    | 226 | G    |
| 35  | 1a    | 247 | G    |
| 35  | 1a    | 251 | G    |
| 35  | 1a    | 266 | G    |
| 35  | 1a    | 267 | C    |
| 35  | 1a    | 281 | G    |
| 35  | 1a    | 282 | A    |
| 35  | 1a    | 283 | U    |
| 35  | 1a    | 289 | G    |
| 35  | 1a    | 306 | A    |
| 35  | 1a    | 328 | C    |
| 35  | 1a    | 345 | C    |
| 35  | 1a    | 347 | G    |
| 35  | 1a    | 351 | G    |
| 35  | 1a    | 352 | C    |
| 35  | 1a    | 367 | U    |
| 35  | 1a    | 372 | C    |
| 35  | 1a    | 392 | C    |
| 35  | 1a    | 397 | A    |
| 35  | 1a    | 406 | G    |
| 35  | 1a    | 413 | G    |
| 35  | 1a    | 422 | C    |
| 35  | 1a    | 424 | G    |
| 35  | 1a    | 429 | U    |
| 35  | 1a    | 439 | U    |
| 35  | 1a    | 467 | U    |
| 35  | 1a    | 479 | U    |
| 35  | 1a    | 482 | A    |
| 35  | 1a    | 484 | G    |
| 35  | 1a    | 485 | U    |
| 35  | 1a    | 486 | U    |
| 35  | 1a    | 496 | A    |
| 35  | 1a    | 497 | G    |
| 35  | 1a    | 527 | 7MG  |
| 35  | 1a    | 530 | G    |
| 35  | 1a    | 531 | U    |
| 35  | 1a    | 532 | A    |
| 35  | 1a    | 533 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | 1a    | 547 | A    |
| 35  | 1a    | 561 | U    |
| 35  | 1a    | 564 | C    |
| 35  | 1a    | 572 | A    |
| 35  | 1a    | 573 | A    |
| 35  | 1a    | 575 | G    |
| 35  | 1a    | 576 | C    |
| 35  | 1a    | 577 | G    |
| 35  | 1a    | 633 | G    |
| 35  | 1a    | 642 | A    |
| 35  | 1a    | 665 | A    |
| 35  | 1a    | 688 | G    |
| 35  | 1a    | 702 | A    |
| 35  | 1a    | 703 | G    |
| 35  | 1a    | 723 | U    |
| 35  | 1a    | 724 | G    |
| 35  | 1a    | 731 | G    |
| 35  | 1a    | 733 | G    |
| 35  | 1a    | 748 | G    |
| 35  | 1a    | 755 | G    |
| 35  | 1a    | 777 | A    |
| 35  | 1a    | 815 | A    |
| 35  | 1a    | 817 | C    |
| 35  | 1a    | 818 | G    |
| 35  | 1a    | 819 | A    |
| 35  | 1a    | 820 | U    |
| 35  | 1a    | 832 | G    |
| 35  | 1a    | 843 | U    |
| 35  | 1a    | 844 | G    |
| 35  | 1a    | 846 | G    |
| 35  | 1a    | 871 | U    |
| 35  | 1a    | 890 | G    |
| 35  | 1a    | 902 | G    |
| 35  | 1a    | 934 | C    |
| 35  | 1a    | 935 | A    |
| 35  | 1a    | 939 | G    |
| 35  | 1a    | 960 | U    |
| 35  | 1a    | 961 | U    |
| 35  | 1a    | 966 | 2MG  |
| 35  | 1a    | 968 | A    |
| 35  | 1a    | 969 | A    |
| 35  | 1a    | 971 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | 1a    | 975  | A    |
| 35  | 1a    | 976  | G    |
| 35  | 1a    | 977  | A    |
| 35  | 1a    | 992  | U    |
| 35  | 1a    | 993  | G    |
| 35  | 1a    | 1004 | A    |
| 35  | 1a    | 1026 | G    |
| 35  | 1a    | 1028 | C    |
| 35  | 1a    | 1030 | U    |
| 35  | 1a    | 1031 | C    |
| 35  | 1a    | 1033 | G    |
| 35  | 1a    | 1034 | G    |
| 35  | 1a    | 1035 | A    |
| 35  | 1a    | 1053 | G    |
| 35  | 1a    | 1056 | U    |
| 35  | 1a    | 1065 | U    |
| 35  | 1a    | 1085 | U    |
| 35  | 1a    | 1094 | G    |
| 35  | 1a    | 1101 | A    |
| 35  | 1a    | 1130 | A    |
| 35  | 1a    | 1137 | C    |
| 35  | 1a    | 1138 | G    |
| 35  | 1a    | 1139 | G    |
| 35  | 1a    | 1140 | C    |
| 35  | 1a    | 1159 | U    |
| 35  | 1a    | 1168 | U    |
| 35  | 1a    | 1183 | U    |
| 35  | 1a    | 1191 | A    |
| 35  | 1a    | 1196 | A    |
| 35  | 1a    | 1197 | A    |
| 35  | 1a    | 1201 | A    |
| 35  | 1a    | 1202 | U    |
| 35  | 1a    | 1207 | 2MG  |
| 35  | 1a    | 1212 | U    |
| 35  | 1a    | 1213 | A    |
| 35  | 1a    | 1225 | A    |
| 35  | 1a    | 1226 | C    |
| 35  | 1a    | 1227 | A    |
| 35  | 1a    | 1238 | A    |
| 35  | 1a    | 1240 | U    |
| 35  | 1a    | 1241 | G    |
| 35  | 1a    | 1256 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | 1a    | 1258 | G    |
| 35  | 1a    | 1260 | G    |
| 35  | 1a    | 1278 | G    |
| 35  | 1a    | 1280 | A    |
| 35  | 1a    | 1281 | C    |
| 35  | 1a    | 1282 | C    |
| 35  | 1a    | 1287 | A    |
| 35  | 1a    | 1298 | U    |
| 35  | 1a    | 1300 | G    |
| 35  | 1a    | 1301 | U    |
| 35  | 1a    | 1302 | C    |
| 35  | 1a    | 1317 | C    |
| 35  | 1a    | 1323 | G    |
| 35  | 1a    | 1346 | A    |
| 35  | 1a    | 1347 | G    |
| 35  | 1a    | 1348 | U    |
| 35  | 1a    | 1363 | A    |
| 35  | 1a    | 1395 | C    |
| 35  | 1a    | 1398 | A    |
| 35  | 1a    | 1400 | C    |
| 35  | 1a    | 1402 | 4OC  |
| 35  | 1a    | 1403 | C    |
| 35  | 1a    | 1407 | 5MC  |
| 35  | 1a    | 1433 | A    |
| 35  | 1a    | 1446 | A    |
| 35  | 1a    | 1448 | C    |
| 35  | 1a    | 1452 | C    |
| 35  | 1a    | 1491 | G    |
| 35  | 1a    | 1492 | A    |
| 35  | 1a    | 1494 | G    |
| 35  | 1a    | 1497 | G    |
| 35  | 1a    | 1498 | UR3  |
| 35  | 1a    | 1499 | A    |
| 35  | 1a    | 1502 | A    |
| 35  | 1a    | 1506 | U    |
| 35  | 1a    | 1517 | G    |
| 35  | 1a    | 1520 | C    |
| 35  | 1a    | 1529 | G    |
| 35  | 1a    | 1530 | G    |
| 35  | 1a    | 1533 | C    |
| 35  | 1a    | 1534 | A    |
| 35  | 1a    | 1535 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | 1a    | 1536 | C    |
| 58  | 1x    | 9    | A    |
| 58  | 1x    | 19   | G    |
| 58  | 1x    | 22   | G    |
| 58  | 1x    | 47   | U    |
| 58  | 1x    | 67   | A    |

All (35) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 51   | G    |
| 1   | 1A    | 86   | G    |
| 1   | 1A    | 204  | A    |
| 1   | 1A    | 242  | G    |
| 1   | 1A    | 372  | G    |
| 1   | 1A    | 458  | G    |
| 1   | 1A    | 479  | A    |
| 1   | 1A    | 490  | C    |
| 1   | 1A    | 747  | 5MU  |
| 1   | 1A    | 752  | A    |
| 1   | 1A    | 858  | G    |
| 1   | 1A    | 859  | G    |
| 1   | 1A    | 1020 | A    |
| 1   | 1A    | 1022 | G    |
| 1   | 1A    | 1070 | A    |
| 1   | 1A    | 1111 | A    |
| 1   | 1A    | 1130 | U    |
| 1   | 1A    | 1182 | G    |
| 1   | 1A    | 1190 | G    |
| 1   | 1A    | 1300 | G    |
| 1   | 1A    | 1378 | A    |
| 1   | 1A    | 1399 | C    |
| 1   | 1A    | 1432 | G    |
| 1   | 1A    | 1940 | U    |
| 1   | 1A    | 2251 | OMG  |
| 1   | 1A    | 2286 | G    |
| 1   | 1A    | 2326 | C    |
| 1   | 1A    | 2333 | A    |
| 1   | 1A    | 2391 | G    |
| 1   | 1A    | 2566 | A    |
| 1   | 1A    | 2655 | G    |
| 1   | 1A    | 2756 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2808 | G    |
| 2   | 1B    | 66   | A    |
| 2   | 1B    | 88   | C    |

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

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 1   | PSU  | 1A    | 2580 | 1    | 18,21,22     | 1.38 | 2 (11%)     | 21,30,33    | 2.23 | 3 (14%)     |
| 1   | PSU  | 1A    | 746  | 1    | 18,21,22     | 1.48 | 3 (16%)     | 21,30,33    | 2.11 | 4 (19%)     |
| 35  | 2MG  | 1a    | 1516 | 35   | 23,26,27     | 1.28 | 2 (8%)      | 33,38,41    | 2.04 | 6 (18%)     |
| 1   | 2MG  | 1A    | 2445 | 1    | 23,26,27     | 1.23 | 3 (13%)     | 33,38,41    | 2.14 | 7 (21%)     |
| 1   | PSU  | 1A    | 1917 | 1    | 18,21,22     | 1.39 | 2 (11%)     | 21,30,33    | 2.14 | 3 (14%)     |
| 1   | 1MG  | 1A    | 745  | 1    | 23,26,27     | 1.25 | 2 (8%)      | 33,39,42    | 1.82 | 5 (15%)     |
| 35  | 5MC  | 1a    | 1407 | 35   | 19,22,23     | 1.54 | 3 (15%)     | 26,32,35    | 1.11 | 2 (7%)      |
| 35  | MA6  | 1a    | 1519 | 35   | 23,26,27     | 1.52 | 4 (17%)     | 33,38,41    | 2.40 | 12 (36%)    |
| 1   | PSU  | 1A    | 2604 | 1    | 18,21,22     | 1.40 | 2 (11%)     | 21,30,33    | 2.19 | 3 (14%)     |
| 35  | 5MC  | 1a    | 967  | 35   | 19,22,23     | 1.77 | 3 (15%)     | 26,32,35    | 1.40 | 4 (15%)     |
| 1   | OMC  | 1A    | 2498 | 1    | 19,22,23     | 0.81 | 0           | 25,31,34    | 0.94 | 1 (4%)      |
| 1   | 5MC  | 1A    | 1962 | 1    | 19,22,23     | 1.65 | 3 (15%)     | 26,32,35    | 1.34 | 4 (15%)     |
| 1   | 2MG  | 1A    | 1835 | 1    | 23,26,27     | 1.29 | 4 (17%)     | 33,38,41    | 2.16 | 5 (15%)     |
| 1   | PSU  | 1A    | 2504 | 1    | 18,21,22     | 1.41 | 2 (11%)     | 21,30,33    | 2.19 | 4 (19%)     |
| 1   | 5MU  | 1A    | 747  | 1    | 19,22,23     | 1.50 | 5 (26%)     | 27,32,35    | 2.51 | 8 (29%)     |
| 35  | 2MG  | 1a    | 966  | 35   | 23,26,27     | 1.30 | 4 (17%)     | 33,38,41    | 2.09 | 5 (15%)     |
| 1   | 5MU  | 1A    | 1939 | 1    | 19,22,23     | 1.46 | 6 (31%)     | 27,32,35    | 2.22 | 6 (22%)     |
| 1   | 6MZ  | 1A    | 1618 | 1    | 22,25,26     | 1.48 | 5 (22%)     | 29,36,39    | 2.17 | 10 (34%)    |
| 35  | 7MG  | 1a    | 527  | 35   | 23,26,27     | 1.55 | 3 (13%)     | 27,39,42    | 2.63 | 8 (29%)     |
| 35  | 2MG  | 1a    | 1207 | 35   | 23,26,27     | 1.25 | 4 (17%)     | 33,38,41    | 2.18 | 5 (15%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMG  | 1A    | 2251 | 1,58 | 23,26,27     | 1.17 | 3 (13%)  | 32,38,41    | 2.00 | 6 (18%)  |
| 1   | PSU  | 1A    | 2605 | 1    | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 2.13 | 3 (14%)  |
| 1   | 6MZ  | 1A    | 2030 | 1    | 22,25,26     | 1.55 | 4 (18%)  | 29,36,39    | 2.39 | 10 (34%) |
| 58  | PSU  | 1x    | 55   | 58   | 18,21,22     | 1.39 | 2 (11%)  | 21,30,33    | 2.10 | 5 (23%)  |
| 1   | 3TD  | 1A    | 1915 | 1    | 19,22,23     | 1.51 | 5 (26%)  | 23,32,35    | 2.30 | 6 (26%)  |
| 35  | UR3  | 1a    | 1498 | 35   | 19,22,23     | 1.07 | 2 (10%)  | 26,32,35    | 1.82 | 6 (23%)  |
| 1   | G7M  | 1A    | 2069 | 1    | 23,26,27     | 1.58 | 3 (13%)  | 34,39,42    | 1.85 | 6 (17%)  |
| 1   | H2U  | 1A    | 2449 | 1    | 18,21,22     | 1.12 | 2 (11%)  | 19,30,33    | 1.37 | 2 (10%)  |
| 58  | 7MG  | 1x    | 46   | 58   | 23,26,27     | 1.29 | 2 (8%)   | 27,39,42    | 2.77 | 7 (25%)  |
| 35  | MA6  | 1a    | 1518 | 35   | 23,26,27     | 1.57 | 4 (17%)  | 33,38,41    | 2.42 | 12 (36%) |
| 35  | PSU  | 1a    | 516  | 35   | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 2.20 | 3 (14%)  |
| 58  | PSU  | 1x    | 65   | 58   | 18,21,22     | 1.38 | 3 (16%)  | 21,30,33    | 2.14 | 4 (19%)  |
| 1   | OMU  | 1A    | 2552 | 1    | 19,22,23     | 1.28 | 3 (15%)  | 25,31,34    | 1.92 | 6 (24%)  |
| 1   | PSU  | 1A    | 955  | 1    | 18,21,22     | 1.42 | 2 (11%)  | 21,30,33    | 2.21 | 3 (14%)  |
| 1   | 2MA  | 1A    | 2503 | 1    | 22,25,26     | 1.55 | 5 (22%)  | 32,37,40    | 2.49 | 9 (28%)  |
| 1   | PSU  | 1A    | 1911 | 1    | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 2.21 | 3 (14%)  |
| 35  | 4OC  | 1a    | 1402 | 35   | 20,23,24     | 0.88 | 0        | 25,32,35    | 1.46 | 4 (16%)  |
| 1   | PSU  | 1A    | 2457 | 1    | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 2.29 | 4 (19%)  |
| 58  | 5MU  | 1x    | 54   | 58   | 19,22,23     | 1.40 | 6 (31%)  | 27,32,35    | 2.16 | 8 (29%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 1   | PSU  | 1A    | 2580 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 746  | 1    | -       | 2/7/25/26  | 0/2/2/2 |
| 35  | 2MG  | 1a    | 1516 | 35   | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | 2MG  | 1A    | 2445 | 1    | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 1A    | 1917 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 1MG  | 1A    | 745  | 1    | -       | 0/7/25/26  | 0/3/3/3 |
| 35  | 5MC  | 1a    | 1407 | 35   | -       | 2/7/25/26  | 0/2/2/2 |
| 35  | MA6  | 1a    | 1519 | 35   | -       | 1/11/29/30 | 0/3/3/3 |
| 1   | PSU  | 1A    | 2604 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 35  | 5MC  | 1a    | 967  | 35   | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | 1A    | 2498 | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1962 | 1    | -       | 4/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 1   | 2MG  | 1A    | 1835 | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 1A    | 2504 | 1    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 747  | 1    | -       | 4/7/25/26  | 0/2/2/2 |
| 35  | 2MG  | 1a    | 966  | 35   | -       | 3/9/27/28  | 0/3/3/3 |
| 1   | 5MU  | 1A    | 1939 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 6MZ  | 1A    | 1618 | 1    | -       | 2/9/27/28  | 0/3/3/3 |
| 35  | 7MG  | 1a    | 527  | 35   | -       | 3/7/37/38  | 0/3/3/3 |
| 35  | 2MG  | 1a    | 1207 | 35   | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | OMG  | 1A    | 2251 | 1,58 | -       | 4/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 1A    | 2605 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 6MZ  | 1A    | 2030 | 1    | -       | 2/9/27/28  | 0/3/3/3 |
| 58  | PSU  | 1x    | 55   | 58   | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | 3TD  | 1A    | 1915 | 1    | -       | 3/7/25/26  | 0/2/2/2 |
| 35  | UR3  | 1a    | 1498 | 35   | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | G7M  | 1A    | 2069 | 1    | -       | 2/7/25/26  | 0/3/3/3 |
| 1   | H2U  | 1A    | 2449 | 1    | -       | 0/7/38/39  | 0/2/2/2 |
| 58  | 7MG  | 1x    | 46   | 58   | -       | 2/7/37/38  | 0/3/3/3 |
| 35  | MA6  | 1a    | 1518 | 35   | -       | 2/11/29/30 | 0/3/3/3 |
| 35  | PSU  | 1a    | 516  | 35   | -       | 0/7/25/26  | 0/2/2/2 |
| 58  | PSU  | 1x    | 65   | 58   | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | 1A    | 2552 | 1    | -       | 3/9/27/28  | 0/2/2/2 |
| 1   | PSU  | 1A    | 955  | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 2MA  | 1A    | 2503 | 1    | -       | 3/7/25/26  | 0/3/3/3 |
| 1   | PSU  | 1A    | 1911 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 35  | 4OC  | 1a    | 1402 | 35   | -       | 3/9/29/30  | 0/2/2/2 |
| 1   | PSU  | 1A    | 2457 | 1    | -       | 2/7/25/26  | 0/2/2/2 |
| 58  | 5MU  | 1x    | 54   | 58   | -       | 0/7/25/26  | 0/2/2/2 |

All (116) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 35  | 1a    | 967  | 5MC  | C5-C4 | 6.47  | 1.49        | 1.44     |
| 1   | 1A    | 1962 | 5MC  | C5-C4 | 6.04  | 1.48        | 1.44     |
| 35  | 1a    | 1407 | 5MC  | C5-C4 | 5.55  | 1.48        | 1.44     |
| 1   | 1A    | 2069 | G7M  | C5-N7 | -5.10 | 1.33        | 1.39     |
| 1   | 1A    | 2030 | 6MZ  | C5-C4 | 5.00  | 1.48        | 1.39     |
| 1   | 1A    | 2503 | 2MA  | C5-C4 | 4.86  | 1.47        | 1.39     |
| 35  | 1a    | 1518 | MA6  | C5-C4 | 4.79  | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | 1a    | 1519 | MA6  | C5-C4   | 4.79  | 1.47        | 1.39     |
| 1   | 1A    | 1618 | 6MZ  | C5-C4   | 4.69  | 1.47        | 1.39     |
| 35  | 1a    | 527  | 7MG  | C4-N9   | -4.63 | 1.32        | 1.37     |
| 1   | 1A    | 2605 | PSU  | C6-C5   | 3.93  | 1.39        | 1.35     |
| 58  | 1x    | 55   | PSU  | C6-C5   | 3.92  | 1.39        | 1.35     |
| 1   | 1A    | 955  | PSU  | C6-C5   | 3.81  | 1.39        | 1.35     |
| 1   | 1A    | 2504 | PSU  | C6-C5   | 3.79  | 1.39        | 1.35     |
| 1   | 1A    | 2604 | PSU  | C6-C5   | 3.74  | 1.39        | 1.35     |
| 35  | 1a    | 516  | PSU  | C6-C5   | 3.70  | 1.39        | 1.35     |
| 1   | 1A    | 2580 | PSU  | C6-C5   | 3.68  | 1.39        | 1.35     |
| 1   | 1A    | 1917 | PSU  | C6-C5   | 3.65  | 1.39        | 1.35     |
| 1   | 1A    | 1911 | PSU  | C6-C5   | 3.62  | 1.39        | 1.35     |
| 1   | 1A    | 2457 | PSU  | C6-C5   | 3.56  | 1.39        | 1.35     |
| 58  | 1x    | 46   | 7MG  | C5-C4   | 3.47  | 1.48        | 1.37     |
| 1   | 1A    | 747  | 5MU  | C6-C5   | 3.45  | 1.40        | 1.34     |
| 1   | 1A    | 745  | 1MG  | C5-C4   | 3.42  | 1.48        | 1.38     |
| 1   | 1A    | 746  | PSU  | C6-C5   | 3.37  | 1.39        | 1.35     |
| 35  | 1a    | 1516 | 2MG  | C5-C4   | 3.33  | 1.47        | 1.38     |
| 35  | 1a    | 527  | 7MG  | C5-C4   | 3.30  | 1.47        | 1.37     |
| 1   | 1A    | 1915 | 3TD  | C6-C5   | 3.30  | 1.38        | 1.35     |
| 35  | 1a    | 1518 | MA6  | C5-C6   | 3.23  | 1.49        | 1.41     |
| 35  | 1a    | 966  | 2MG  | C5-C4   | 3.19  | 1.47        | 1.38     |
| 1   | 1A    | 746  | PSU  | O4'-C1' | -3.18 | 1.39        | 1.43     |
| 1   | 1A    | 2069 | G7M  | C5-C4   | 3.18  | 1.46        | 1.38     |
| 1   | 1A    | 1915 | 3TD  | C4-N3   | -3.17 | 1.33        | 1.40     |
| 1   | 1A    | 2445 | 2MG  | C5-C4   | 3.15  | 1.47        | 1.38     |
| 1   | 1A    | 1835 | 2MG  | C5-C4   | 3.12  | 1.47        | 1.38     |
| 35  | 1a    | 1207 | 2MG  | C5-C4   | 3.09  | 1.47        | 1.38     |
| 1   | 1A    | 2030 | 6MZ  | C5-C6   | 3.06  | 1.49        | 1.41     |
| 1   | 1A    | 2552 | OMU  | C4-N3   | -3.01 | 1.33        | 1.38     |
| 1   | 1A    | 2251 | OMG  | C5-C4   | 2.97  | 1.46        | 1.38     |
| 58  | 1x    | 65   | PSU  | C6-C5   | 2.95  | 1.38        | 1.35     |
| 1   | 1A    | 2449 | H2U  | C2-N3   | -2.94 | 1.32        | 1.38     |
| 1   | 1A    | 1917 | PSU  | C4-N3   | -2.92 | 1.33        | 1.38     |
| 1   | 1A    | 955  | PSU  | C4-N3   | -2.92 | 1.33        | 1.38     |
| 1   | 1A    | 2504 | PSU  | C4-N3   | -2.90 | 1.33        | 1.38     |
| 1   | 1A    | 1835 | 2MG  | C6-N1   | -2.88 | 1.33        | 1.38     |
| 35  | 1a    | 1519 | MA6  | C5-C6   | 2.88  | 1.48        | 1.41     |
| 1   | 1A    | 1911 | PSU  | C4-N3   | -2.88 | 1.33        | 1.38     |
| 1   | 1A    | 747  | 5MU  | C4-N3   | -2.88 | 1.33        | 1.38     |
| 1   | 1A    | 2457 | PSU  | C4-N3   | -2.86 | 1.33        | 1.38     |
| 1   | 1A    | 2605 | PSU  | C4-N3   | -2.86 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | 1a    | 516  | PSU  | C4-N3   | -2.85 | 1.33        | 1.38     |
| 1   | 1A    | 2604 | PSU  | C4-N3   | -2.85 | 1.33        | 1.38     |
| 1   | 1A    | 1939 | 5MU  | C4-N3   | -2.84 | 1.33        | 1.38     |
| 1   | 1A    | 2580 | PSU  | C4-N3   | -2.84 | 1.33        | 1.38     |
| 1   | 1A    | 1939 | 5MU  | C6-C5   | 2.81  | 1.39        | 1.34     |
| 35  | 1a    | 966  | 2MG  | C6-N1   | -2.80 | 1.33        | 1.38     |
| 58  | 1x    | 55   | PSU  | C4-N3   | -2.80 | 1.33        | 1.38     |
| 1   | 1A    | 745  | 1MG  | C2-N1   | 2.79  | 1.42        | 1.37     |
| 1   | 1A    | 2503 | 2MA  | C5-C6   | 2.77  | 1.48        | 1.41     |
| 58  | 1x    | 54   | 5MU  | C4-N3   | -2.75 | 1.33        | 1.38     |
| 35  | 1a    | 1498 | UR3  | C2-N1   | 2.74  | 1.42        | 1.38     |
| 35  | 1a    | 1518 | MA6  | C8-N7   | 2.68  | 1.36        | 1.31     |
| 1   | 1A    | 1618 | 6MZ  | C5-C6   | 2.67  | 1.48        | 1.41     |
| 1   | 1A    | 2449 | H2U  | C4-N3   | -2.62 | 1.33        | 1.37     |
| 58  | 1x    | 65   | PSU  | C4-N3   | -2.62 | 1.33        | 1.38     |
| 35  | 1a    | 967  | 5MC  | C6-C5   | 2.60  | 1.38        | 1.34     |
| 1   | 1A    | 1915 | 3TD  | O4'-C1' | -2.60 | 1.40        | 1.43     |
| 35  | 1a    | 1207 | 2MG  | C6-N1   | -2.50 | 1.34        | 1.38     |
| 1   | 1A    | 2030 | 6MZ  | C8-N7   | 2.50  | 1.36        | 1.31     |
| 1   | 1A    | 746  | PSU  | C4-N3   | -2.49 | 1.34        | 1.38     |
| 1   | 1A    | 2445 | 2MG  | C6-N1   | -2.48 | 1.34        | 1.38     |
| 1   | 1A    | 2069 | G7M  | C6-N1   | -2.46 | 1.34        | 1.38     |
| 1   | 1A    | 1939 | 5MU  | C4-C5   | 2.45  | 1.48        | 1.44     |
| 58  | 1x    | 54   | 5MU  | C2-N1   | 2.45  | 1.42        | 1.38     |
| 58  | 1x    | 54   | 5MU  | C6-C5   | 2.44  | 1.38        | 1.34     |
| 58  | 1x    | 54   | 5MU  | C6-N1   | -2.42 | 1.33        | 1.38     |
| 58  | 1x    | 46   | 7MG  | C6-N1   | -2.41 | 1.34        | 1.38     |
| 58  | 1x    | 65   | PSU  | O4'-C1' | -2.40 | 1.40        | 1.43     |
| 35  | 1a    | 967  | 5MC  | C6-N1   | -2.38 | 1.34        | 1.38     |
| 1   | 1A    | 2503 | 2MA  | C8-N7   | 2.38  | 1.36        | 1.31     |
| 1   | 1A    | 1962 | 5MC  | C6-N1   | -2.37 | 1.34        | 1.38     |
| 35  | 1a    | 966  | 2MG  | C2-N3   | 2.34  | 1.36        | 1.32     |
| 1   | 1A    | 1962 | 5MC  | C6-C5   | 2.32  | 1.38        | 1.34     |
| 35  | 1a    | 1519 | MA6  | C5-N7   | -2.32 | 1.34        | 1.39     |
| 35  | 1a    | 1407 | 5MC  | C6-N1   | -2.32 | 1.34        | 1.38     |
| 1   | 1A    | 1939 | 5MU  | C6-N1   | -2.30 | 1.34        | 1.38     |
| 35  | 1a    | 527  | 7MG  | C6-N1   | -2.30 | 1.34        | 1.38     |
| 1   | 1A    | 1618 | 6MZ  | C8-N7   | 2.29  | 1.36        | 1.31     |
| 35  | 1a    | 1516 | 2MG  | C6-N1   | -2.29 | 1.34        | 1.38     |
| 1   | 1A    | 2251 | OMG  | C6-N1   | -2.29 | 1.34        | 1.38     |
| 35  | 1a    | 1407 | 5MC  | C6-C5   | 2.29  | 1.38        | 1.34     |
| 1   | 1A    | 1939 | 5MU  | C2-N1   | 2.28  | 1.42        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | 1A    | 1939 | 5MU  | C2-N3 | -2.27 | 1.34        | 1.38     |
| 1   | 1A    | 747  | 5MU  | C4-C5 | 2.24  | 1.48        | 1.44     |
| 1   | 1A    | 1618 | 6MZ  | C4-N9 | -2.20 | 1.33        | 1.37     |
| 35  | 1a    | 1519 | MA6  | C8-N7 | 2.20  | 1.35        | 1.31     |
| 1   | 1A    | 747  | 5MU  | C2-N1 | 2.20  | 1.41        | 1.38     |
| 1   | 1A    | 1835 | 2MG  | C2-N3 | 2.19  | 1.36        | 1.32     |
| 35  | 1a    | 966  | 2MG  | C5-N7 | -2.19 | 1.34        | 1.39     |
| 1   | 1A    | 1618 | 6MZ  | C5-N7 | -2.18 | 1.35        | 1.39     |
| 1   | 1A    | 747  | 5MU  | C2-N3 | -2.15 | 1.34        | 1.38     |
| 35  | 1a    | 1207 | 2MG  | C2-N3 | 2.15  | 1.36        | 1.32     |
| 58  | 1x    | 54   | 5MU  | C4-C5 | 2.14  | 1.48        | 1.44     |
| 1   | 1A    | 2030 | 6MZ  | C5-N7 | -2.12 | 1.35        | 1.39     |
| 35  | 1a    | 1207 | 2MG  | C5-N7 | -2.11 | 1.34        | 1.39     |
| 1   | 1A    | 2552 | OMU  | C5-C4 | -2.09 | 1.39        | 1.43     |
| 1   | 1A    | 2445 | 2MG  | C2-N3 | 2.08  | 1.35        | 1.32     |
| 35  | 1a    | 1518 | MA6  | C5-N7 | -2.07 | 1.35        | 1.39     |
| 1   | 1A    | 1835 | 2MG  | C5-N7 | -2.07 | 1.34        | 1.39     |
| 1   | 1A    | 2552 | OMU  | C2-N3 | -2.07 | 1.34        | 1.38     |
| 1   | 1A    | 2251 | OMG  | C5-N7 | -2.05 | 1.35        | 1.39     |
| 1   | 1A    | 2503 | 2MA  | C4-N9 | -2.04 | 1.33        | 1.37     |
| 35  | 1a    | 1498 | UR3  | C6-C5 | 2.03  | 1.39        | 1.35     |
| 1   | 1A    | 2503 | 2MA  | C5-N7 | -2.02 | 1.35        | 1.39     |
| 1   | 1A    | 1915 | 3TD  | C2-N1 | -2.02 | 1.34        | 1.37     |
| 1   | 1A    | 1915 | 3TD  | C2-N3 | -2.01 | 1.34        | 1.38     |
| 58  | 1x    | 54   | 5MU  | C2-N3 | -2.01 | 1.34        | 1.38     |

All (212) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 58  | 1x    | 46   | 7MG  | N9-C4-N3 | 9.74  | 139.74      | 125.46   |
| 1   | 1A    | 2503 | 2MA  | C5-C4-N3 | -8.41 | 118.32      | 127.18   |
| 35  | 1a    | 527  | 7MG  | N9-C4-N3 | 8.39  | 137.76      | 125.46   |
| 1   | 1A    | 1915 | 3TD  | N1-C2-N3 | 8.09  | 122.01      | 116.13   |
| 1   | 1A    | 2457 | PSU  | N1-C2-N3 | 6.96  | 122.51      | 115.17   |
| 1   | 1A    | 2580 | PSU  | N1-C2-N3 | 6.89  | 122.43      | 115.17   |
| 1   | 1A    | 1835 | 2MG  | C2-N3-C4 | 6.78  | 120.48      | 112.00   |
| 35  | 1a    | 516  | PSU  | N1-C2-N3 | 6.76  | 122.30      | 115.17   |
| 1   | 1A    | 1911 | PSU  | N1-C2-N3 | 6.75  | 122.29      | 115.17   |
| 1   | 1A    | 955  | PSU  | N1-C2-N3 | 6.75  | 122.29      | 115.17   |
| 1   | 1A    | 2504 | PSU  | N1-C2-N3 | 6.73  | 122.27      | 115.17   |
| 1   | 1A    | 2604 | PSU  | N1-C2-N3 | 6.72  | 122.26      | 115.17   |
| 35  | 1a    | 1516 | 2MG  | C2-N3-C4 | 6.69  | 120.38      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | 1A    | 2503 | 2MA  | N3-C4-N9  | 6.64  | 135.41      | 126.99   |
| 1   | 1A    | 1917 | PSU  | N1-C2-N3  | 6.56  | 122.09      | 115.17   |
| 35  | 1a    | 966  | 2MG  | C2-N3-C4  | 6.54  | 120.18      | 112.00   |
| 1   | 1A    | 2605 | PSU  | N1-C2-N3  | 6.51  | 122.04      | 115.17   |
| 35  | 1a    | 1207 | 2MG  | C2-N3-C4  | 6.48  | 120.11      | 112.00   |
| 1   | 1A    | 2445 | 2MG  | C2-N3-C4  | 6.47  | 120.09      | 112.00   |
| 35  | 1a    | 1498 | UR3  | C4-N3-C2  | -6.46 | 119.38      | 124.58   |
| 58  | 1x    | 55   | PSU  | N1-C2-N3  | 6.43  | 121.95      | 115.17   |
| 58  | 1x    | 65   | PSU  | N1-C2-N3  | 6.41  | 121.93      | 115.17   |
| 35  | 1a    | 527  | 7MG  | N9-C8-N7  | -6.24 | 94.54       | 103.37   |
| 1   | 1A    | 746  | PSU  | N1-C2-N3  | 6.15  | 121.65      | 115.17   |
| 1   | 1A    | 747  | 5MU  | N3-C2-N1  | 6.04  | 122.75      | 114.89   |
| 1   | 1A    | 1835 | 2MG  | C5-C4-N3  | -6.04 | 118.78      | 128.39   |
| 35  | 1a    | 1518 | MA6  | C5-C4-N3  | -6.03 | 118.42      | 126.72   |
| 35  | 1a    | 966  | 2MG  | C5-C4-N3  | -5.94 | 118.93      | 128.39   |
| 35  | 1a    | 1519 | MA6  | C5-C4-N3  | -5.91 | 118.57      | 126.72   |
| 58  | 1x    | 46   | 7MG  | C5-C4-N3  | -5.82 | 117.21      | 128.13   |
| 1   | 1A    | 747  | 5MU  | C4-N3-C2  | -5.81 | 119.72      | 127.34   |
| 1   | 1A    | 2030 | 6MZ  | C5-C4-N3  | -5.80 | 118.73      | 126.72   |
| 35  | 1a    | 1207 | 2MG  | C5-C4-N3  | -5.74 | 119.25      | 128.39   |
| 1   | 1A    | 745  | 1MG  | C5-C4-N3  | -5.68 | 119.36      | 128.39   |
| 1   | 1A    | 2445 | 2MG  | C5-C4-N3  | -5.65 | 119.40      | 128.39   |
| 1   | 1A    | 2069 | G7M  | N9-C4-N3  | 5.65  | 137.24      | 125.95   |
| 1   | 1A    | 2251 | OMG  | C5-C4-N3  | -5.59 | 119.50      | 128.39   |
| 1   | 1A    | 2069 | G7M  | C5-C4-N3  | -5.54 | 117.68      | 128.15   |
| 1   | 1A    | 1939 | 5MU  | C4-N3-C2  | -5.40 | 120.27      | 127.34   |
| 35  | 1a    | 1516 | 2MG  | C5-C4-N3  | -5.38 | 119.82      | 128.39   |
| 1   | 1A    | 2030 | 6MZ  | C9-N6-C6  | -5.29 | 117.94      | 122.85   |
| 1   | 1A    | 1939 | 5MU  | N3-C2-N1  | 5.28  | 121.76      | 114.89   |
| 1   | 1A    | 1618 | 6MZ  | C5-C4-N3  | -5.16 | 119.61      | 126.72   |
| 1   | 1A    | 2552 | OMU  | C4-N3-C2  | -5.14 | 120.24      | 126.61   |
| 35  | 1a    | 527  | 7MG  | C5-C4-N3  | -5.12 | 118.52      | 128.13   |
| 58  | 1x    | 54   | 5MU  | C4-N3-C2  | -5.08 | 120.68      | 127.34   |
| 35  | 1a    | 1519 | MA6  | C10-N6-C6 | -4.99 | 107.83      | 120.52   |
| 1   | 1A    | 2251 | OMG  | C2-N3-C4  | 4.93  | 120.78      | 112.30   |
| 1   | 1A    | 2457 | PSU  | C4-N3-C2  | -4.93 | 119.59      | 126.37   |
| 1   | 1A    | 747  | 5MU  | C5-C6-N1  | -4.92 | 117.97      | 123.31   |
| 58  | 1x    | 46   | 7MG  | N9-C8-N7  | -4.87 | 96.48       | 103.37   |
| 35  | 1a    | 1207 | 2MG  | N9-C4-N3  | 4.82  | 135.59      | 125.95   |
| 35  | 1a    | 966  | 2MG  | N9-C4-N3  | 4.78  | 135.51      | 125.95   |
| 1   | 1A    | 2504 | PSU  | C4-N3-C2  | -4.77 | 119.80      | 126.37   |
| 1   | 1A    | 2580 | PSU  | C4-N3-C2  | -4.77 | 119.80      | 126.37   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 58  | 1x    | 54   | 5MU  | N3-C2-N1  | 4.75  | 121.08      | 114.89   |
| 35  | 1a    | 516  | PSU  | C4-N3-C2  | -4.73 | 119.86      | 126.37   |
| 1   | 1A    | 1911 | PSU  | C4-N3-C2  | -4.70 | 119.90      | 126.37   |
| 1   | 1A    | 2069 | G7M  | C2-N3-C4  | 4.67  | 120.35      | 112.30   |
| 1   | 1A    | 1917 | PSU  | C4-N3-C2  | -4.63 | 119.99      | 126.37   |
| 1   | 1A    | 1939 | 5MU  | C5-C4-N3  | 4.63  | 119.35      | 115.32   |
| 1   | 1A    | 955  | PSU  | C4-N3-C2  | -4.62 | 120.01      | 126.37   |
| 1   | 1A    | 2604 | PSU  | C4-N3-C2  | -4.60 | 120.03      | 126.37   |
| 58  | 1x    | 54   | 5MU  | C5-C4-N3  | 4.59  | 119.32      | 115.32   |
| 1   | 1A    | 1835 | 2MG  | N9-C4-N3  | 4.59  | 135.13      | 125.95   |
| 1   | 1A    | 2605 | PSU  | C4-N3-C2  | -4.58 | 120.06      | 126.37   |
| 1   | 1A    | 745  | 1MG  | N9-C4-N3  | 4.57  | 135.09      | 125.95   |
| 1   | 1A    | 747  | 5MU  | C5-C4-N3  | 4.56  | 119.29      | 115.32   |
| 1   | 1A    | 2445 | 2MG  | N9-C4-N3  | 4.56  | 135.06      | 125.95   |
| 1   | 1A    | 2030 | 6MZ  | C6-C5-N7  | 4.53  | 137.37      | 132.43   |
| 1   | 1A    | 745  | 1MG  | C2-N3-C4  | 4.47  | 122.02      | 111.98   |
| 35  | 1a    | 1519 | MA6  | N3-C4-N9  | 4.46  | 134.74      | 127.17   |
| 35  | 1a    | 1518 | MA6  | C10-N6-C6 | -4.40 | 109.32      | 120.52   |
| 58  | 1x    | 46   | 7MG  | C2-N3-C4  | 4.33  | 119.75      | 112.30   |
| 1   | 1A    | 1618 | 6MZ  | N3-C4-N9  | 4.32  | 134.51      | 127.17   |
| 58  | 1x    | 54   | 5MU  | O4-C4-C5  | -4.31 | 119.99      | 124.92   |
| 1   | 1A    | 2030 | 6MZ  | N3-C4-N9  | 4.31  | 134.49      | 127.17   |
| 58  | 1x    | 65   | PSU  | O2-C2-N1  | -4.29 | 118.37      | 122.79   |
| 58  | 1x    | 55   | PSU  | C4-N3-C2  | -4.28 | 120.47      | 126.37   |
| 35  | 1a    | 1518 | MA6  | C4-C5-N7  | -4.28 | 105.69      | 110.58   |
| 1   | 1A    | 2552 | OMU  | N3-C2-N1  | 4.26  | 120.44      | 114.89   |
| 1   | 1A    | 2457 | PSU  | O2-C2-N1  | -4.26 | 118.40      | 122.79   |
| 35  | 1a    | 1519 | MA6  | C2-N1-C6  | 4.25  | 122.21      | 111.83   |
| 35  | 1a    | 1516 | 2MG  | N9-C4-N3  | 4.22  | 134.40      | 125.95   |
| 35  | 1a    | 1518 | MA6  | C2-N1-C6  | 4.22  | 122.13      | 111.83   |
| 35  | 1a    | 527  | 7MG  | C2-N3-C4  | 4.20  | 119.53      | 112.30   |
| 1   | 1A    | 2251 | OMG  | N9-C4-N3  | 4.16  | 134.27      | 125.95   |
| 1   | 1A    | 747  | 5MU  | O4-C4-C5  | -4.15 | 120.17      | 124.92   |
| 58  | 1x    | 65   | PSU  | C4-N3-C2  | -4.15 | 120.66      | 126.37   |
| 35  | 1a    | 1518 | MA6  | N3-C4-N9  | 4.08  | 134.11      | 127.17   |
| 1   | 1A    | 2604 | PSU  | O2-C2-N1  | -4.08 | 118.58      | 122.79   |
| 1   | 1A    | 2030 | 6MZ  | C4-C5-N7  | -4.03 | 105.97      | 110.58   |
| 1   | 1A    | 1939 | 5MU  | C5-C6-N1  | -4.01 | 118.96      | 123.31   |
| 1   | 1A    | 2503 | 2MA  | C4-C5-N7  | -3.98 | 106.03      | 110.58   |
| 1   | 1A    | 1939 | 5MU  | O4-C4-C5  | -3.98 | 120.36      | 124.92   |
| 1   | 1A    | 1911 | PSU  | O2-C2-N1  | -3.96 | 118.71      | 122.79   |
| 35  | 1a    | 1519 | MA6  | C4-C5-N7  | -3.93 | 106.09      | 110.58   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1A    | 955  | PSU  | O2-C2-N1    | -3.93 | 118.74      | 122.79   |
| 35  | 1a    | 1518 | MA6  | C2-N3-C4    | 3.90  | 121.36      | 111.83   |
| 1   | 1A    | 2580 | PSU  | O2-C2-N1    | -3.87 | 118.79      | 122.79   |
| 1   | 1A    | 746  | PSU  | C4-N3-C2    | -3.86 | 121.05      | 126.37   |
| 1   | 1A    | 1618 | 6MZ  | C6-C5-N7    | 3.86  | 136.64      | 132.43   |
| 1   | 1A    | 2449 | H2U  | N3-C2-N1    | 3.84  | 120.50      | 116.65   |
| 1   | 1A    | 2552 | OMU  | C5-C4-N3    | 3.83  | 120.16      | 114.80   |
| 35  | 1a    | 1519 | MA6  | C2-N3-C4    | 3.82  | 121.16      | 111.83   |
| 1   | 1A    | 1915 | 3TD  | C4-N3-C2    | -3.75 | 120.64      | 124.61   |
| 35  | 1a    | 1402 | 4OC  | C1'-N1-C2   | 3.72  | 126.66      | 118.44   |
| 35  | 1a    | 516  | PSU  | O2-C2-N1    | -3.72 | 118.96      | 122.79   |
| 1   | 1A    | 746  | PSU  | O2-C2-N1    | -3.66 | 119.01      | 122.79   |
| 1   | 1A    | 2030 | 6MZ  | C2-N3-C4    | 3.66  | 120.77      | 111.83   |
| 1   | 1A    | 1618 | 6MZ  | C9-N6-C6    | -3.65 | 119.46      | 122.85   |
| 1   | 1A    | 2504 | PSU  | O2-C2-N1    | -3.60 | 119.07      | 122.79   |
| 1   | 1A    | 1618 | 6MZ  | C4-N9-C8    | 3.55  | 109.46      | 105.74   |
| 1   | 1A    | 2251 | OMG  | C6-C5-N7    | 3.52  | 136.69      | 130.29   |
| 58  | 1x    | 55   | PSU  | O2-C2-N1    | -3.51 | 119.17      | 122.79   |
| 1   | 1A    | 1917 | PSU  | O2-C2-N1    | -3.50 | 119.18      | 122.79   |
| 35  | 1a    | 1407 | 5MC  | C5-C6-N1    | -3.45 | 119.56      | 123.31   |
| 1   | 1A    | 1618 | 6MZ  | C4-C5-N7    | -3.45 | 106.64      | 110.58   |
| 1   | 1A    | 1915 | 3TD  | O4'-C1'-C2' | 3.43  | 109.90      | 105.15   |
| 1   | 1A    | 2503 | 2MA  | C4-N9-C8    | 3.42  | 109.33      | 105.74   |
| 35  | 1a    | 1519 | MA6  | N1-C2-N3    | -3.42 | 123.41      | 128.58   |
| 35  | 1a    | 967  | 5MC  | C5-C6-N1    | -3.39 | 119.64      | 123.31   |
| 1   | 1A    | 2605 | PSU  | O2-C2-N1    | -3.35 | 119.33      | 122.79   |
| 1   | 1A    | 1835 | 2MG  | C6-C5-N7    | 3.35  | 136.38      | 130.29   |
| 35  | 1a    | 1518 | MA6  | N1-C2-N3    | -3.34 | 123.53      | 128.58   |
| 35  | 1a    | 1519 | MA6  | C9-N6-C6    | -3.30 | 112.13      | 120.52   |
| 58  | 1x    | 54   | 5MU  | C5-C6-N1    | -3.26 | 119.77      | 123.31   |
| 1   | 1A    | 747  | 5MU  | O2-C2-N1    | -3.25 | 118.57      | 122.80   |
| 1   | 1A    | 1618 | 6MZ  | C2-N3-C4    | 3.20  | 119.64      | 111.83   |
| 1   | 1A    | 2503 | 2MA  | N6-C6-N1    | 3.14  | 121.27      | 117.03   |
| 35  | 1a    | 527  | 7MG  | C5-C6-N1    | 3.13  | 116.45      | 110.94   |
| 35  | 1a    | 1516 | 2MG  | C6-C5-N7    | 3.12  | 135.97      | 130.29   |
| 1   | 1A    | 2445 | 2MG  | C6-C5-N7    | 3.10  | 135.92      | 130.29   |
| 35  | 1a    | 1498 | UR3  | C5-C4-N3    | 3.08  | 119.09      | 115.04   |
| 1   | 1A    | 1939 | 5MU  | O2-C2-N1    | -3.04 | 118.84      | 122.80   |
| 1   | 1A    | 2552 | OMU  | O2-C2-N1    | -3.01 | 118.87      | 122.80   |
| 1   | 1A    | 2503 | 2MA  | C5-N7-C8    | 3.01  | 108.19      | 103.45   |
| 35  | 1a    | 967  | 5MC  | C1'-N1-C6   | -3.01 | 116.19      | 121.15   |
| 1   | 1A    | 1962 | 5MC  | C5-C4-N3    | -3.01 | 118.67      | 121.75   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | 1a    | 1402 | 4OC  | C1'-N1-C6   | -2.99 | 114.40      | 120.78   |
| 35  | 1a    | 1518 | MA6  | C10-N6-C9   | -2.98 | 106.61      | 116.18   |
| 1   | 1A    | 2449 | H2U  | O2-C2-N1    | -2.95 | 119.55      | 123.10   |
| 1   | 1A    | 2030 | 6MZ  | N1-C2-N3    | -2.90 | 124.19      | 128.58   |
| 1   | 1A    | 1962 | 5MC  | C5-C6-N1    | -2.89 | 120.17      | 123.31   |
| 35  | 1a    | 1518 | MA6  | C5-N7-C8    | 2.88  | 107.98      | 103.45   |
| 35  | 1a    | 1518 | MA6  | C9-N6-C6    | -2.88 | 113.20      | 120.52   |
| 1   | 1A    | 746  | PSU  | O4'-C1'-C2' | 2.86  | 109.10      | 105.15   |
| 1   | 1A    | 2030 | 6MZ  | C5-N7-C8    | 2.84  | 107.92      | 103.45   |
| 35  | 1a    | 966  | 2MG  | C6-C5-N7    | 2.83  | 135.45      | 130.29   |
| 35  | 1a    | 1498 | UR3  | C6-N1-C2    | -2.81 | 119.51      | 121.80   |
| 35  | 1a    | 1519 | MA6  | C5-N7-C8    | 2.80  | 107.84      | 103.45   |
| 1   | 1A    | 1962 | 5MC  | C1'-N1-C6   | -2.79 | 116.56      | 121.15   |
| 35  | 1a    | 1207 | 2MG  | C6-C5-N7    | 2.76  | 135.32      | 130.29   |
| 58  | 1x    | 46   | 7MG  | C5-C6-N1    | 2.73  | 115.74      | 110.94   |
| 58  | 1x    | 65   | PSU  | O4'-C1'-C2' | 2.71  | 108.90      | 105.15   |
| 1   | 1A    | 1618 | 6MZ  | C5-N7-C8    | 2.69  | 107.68      | 103.45   |
| 1   | 1A    | 2503 | 2MA  | C6-C5-N7    | 2.67  | 137.23      | 132.09   |
| 1   | 1A    | 1618 | 6MZ  | N1-C2-N3    | -2.65 | 124.57      | 128.58   |
| 1   | 1A    | 2503 | 2MA  | C2-N1-C6    | 2.64  | 122.17      | 118.10   |
| 1   | 1A    | 2503 | 2MA  | N9-C8-N7    | -2.64 | 110.19      | 113.94   |
| 35  | 1a    | 1402 | 4OC  | O2-C2-N3    | -2.60 | 118.22      | 122.33   |
| 1   | 1A    | 2069 | G7M  | O6-C6-C5    | -2.60 | 122.20      | 128.01   |
| 1   | 1A    | 2030 | 6MZ  | C4-N9-C8    | 2.60  | 108.47      | 105.74   |
| 1   | 1A    | 2498 | OMC  | CM2-O2'-C2' | -2.58 | 107.85      | 114.47   |
| 1   | 1A    | 1962 | 5MC  | CM5-C5-C6   | -2.57 | 119.37      | 122.85   |
| 35  | 1a    | 1207 | 2MG  | O6-C6-C5    | -2.57 | 119.75      | 126.53   |
| 58  | 1x    | 46   | 7MG  | C5-C4-N9    | -2.57 | 103.05      | 106.33   |
| 1   | 1A    | 1835 | 2MG  | C4-C5-N7    | -2.55 | 106.63      | 110.67   |
| 35  | 1a    | 967  | 5MC  | C5-C4-N3    | -2.54 | 119.15      | 121.75   |
| 1   | 1A    | 1618 | 6MZ  | N9-C8-N7    | -2.54 | 110.33      | 113.94   |
| 1   | 1A    | 2251 | OMG  | C4-C5-N7    | -2.53 | 106.67      | 110.67   |
| 1   | 1A    | 2552 | OMU  | O4-C4-C5    | -2.52 | 120.81      | 125.16   |
| 1   | 1A    | 1915 | 3TD  | C5-C6-N1    | -2.51 | 118.66      | 122.14   |
| 35  | 1a    | 1519 | MA6  | C10-N6-C9   | -2.49 | 108.18      | 116.18   |
| 1   | 1A    | 745  | 1MG  | C6-C5-N7    | 2.47  | 134.85      | 129.36   |
| 1   | 1A    | 745  | 1MG  | C4-C5-N7    | -2.43 | 106.81      | 110.67   |
| 35  | 1a    | 1498 | UR3  | C1'-N1-C2   | 2.43  | 121.02      | 117.04   |
| 58  | 1x    | 54   | 5MU  | O2-C2-N1    | -2.40 | 119.68      | 122.80   |
| 35  | 1a    | 1498 | UR3  | O2-C2-N3    | -2.38 | 118.05      | 121.33   |
| 58  | 1x    | 46   | 7MG  | O6-C6-C5    | -2.34 | 121.89      | 127.62   |
| 35  | 1a    | 1518 | MA6  | C6-C5-N7    | 2.32  | 137.14      | 133.43   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | 1a    | 1407 | 5MC  | C5-C4-N3    | -2.32 | 119.38      | 121.75   |
| 58  | 1x    | 54   | 5MU  | C5M-C5-C4   | 2.30  | 121.23      | 118.78   |
| 1   | 1A    | 2445 | 2MG  | C4-C5-N7    | -2.29 | 107.04      | 110.67   |
| 1   | 1A    | 2069 | G7M  | C2'-C1'-N9  | -2.27 | 106.94      | 113.25   |
| 1   | 1A    | 2445 | 2MG  | O6-C6-C5    | -2.26 | 120.58      | 126.53   |
| 1   | 1A    | 1915 | 3TD  | C1'-C5-C4   | 2.24  | 121.01      | 117.61   |
| 35  | 1a    | 966  | 2MG  | C4-C5-N7    | -2.24 | 107.12      | 110.67   |
| 35  | 1a    | 527  | 7MG  | O6-C6-C5    | -2.21 | 122.20      | 127.62   |
| 35  | 1a    | 967  | 5MC  | O2-C2-N3    | -2.21 | 118.85      | 122.33   |
| 1   | 1A    | 1915 | 3TD  | C3'-C2'-C1' | 2.20  | 104.28      | 101.69   |
| 35  | 1a    | 1402 | 4OC  | C6-C5-C4    | 2.19  | 119.64      | 117.00   |
| 1   | 1A    | 2457 | PSU  | C5-C6-N1    | -2.17 | 119.13      | 122.14   |
| 1   | 1A    | 2069 | G7M  | C5-C6-N1    | 2.17  | 116.32      | 111.84   |
| 1   | 1A    | 2030 | 6MZ  | N9-C8-N7    | -2.17 | 110.86      | 113.94   |
| 35  | 1a    | 1519 | MA6  | C4-N9-C8    | 2.16  | 108.01      | 105.74   |
| 1   | 1A    | 2251 | OMG  | O6-C6-C5    | -2.15 | 120.85      | 126.53   |
| 1   | 1A    | 2552 | OMU  | C5-C6-N1    | -2.14 | 118.36      | 121.84   |
| 58  | 1x    | 54   | 5MU  | C1'-N1-C2   | 2.13  | 121.43      | 117.59   |
| 1   | 1A    | 2445 | 2MG  | N1-C2-N2    | 2.13  | 118.74      | 116.56   |
| 35  | 1a    | 1516 | 2MG  | C4-C5-N7    | -2.12 | 107.31      | 110.67   |
| 1   | 1A    | 747  | 5MU  | C1'-N1-C6   | 2.09  | 124.60      | 121.15   |
| 35  | 1a    | 1519 | MA6  | C6-C5-N7    | 2.09  | 136.77      | 133.43   |
| 58  | 1x    | 55   | PSU  | C6-C5-C4    | -2.06 | 116.78      | 118.17   |
| 35  | 1a    | 527  | 7MG  | C5-C4-N9    | -2.05 | 103.71      | 106.33   |
| 35  | 1a    | 1498 | UR3  | C3U-N3-C4   | 2.05  | 120.71      | 117.87   |
| 1   | 1A    | 2504 | PSU  | C5-C6-N1    | -2.04 | 119.31      | 122.14   |
| 1   | 1A    | 747  | 5MU  | C2'-C3'-C4' | 2.04  | 106.55      | 102.61   |
| 35  | 1a    | 527  | 7MG  | C6-C5-N7    | 2.04  | 135.09      | 131.93   |
| 35  | 1a    | 1516 | 2MG  | O6-C6-C5    | -2.04 | 121.15      | 126.53   |
| 35  | 1a    | 1518 | MA6  | N1-C6-N6    | 2.03  | 119.32      | 116.86   |
| 58  | 1x    | 55   | PSU  | O4'-C1'-C2' | 2.02  | 107.94      | 105.15   |

There are no chirality outliers.

All (56) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | 1A    | 746  | PSU  | O4'-C4'-C5'-O5' |
| 1   | 1A    | 747  | 5MU  | C2'-C1'-N1-C2   |
| 1   | 1A    | 747  | 5MU  | C2'-C1'-N1-C6   |
| 1   | 1A    | 1618 | 6MZ  | C5-C6-N6-C9     |
| 1   | 1A    | 1618 | 6MZ  | N1-C6-N6-C9     |
| 1   | 1A    | 1915 | 3TD  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | 1A    | 1962 | 5MC  | O4'-C4'-C5'-O5' |
| 1   | 1A    | 2251 | OMG  | O4'-C4'-C5'-O5' |
| 1   | 1A    | 2251 | OMG  | C3'-C4'-C5'-O5' |
| 1   | 1A    | 2251 | OMG  | C1'-C2'-O2'-CM2 |
| 1   | 1A    | 2504 | PSU  | O4'-C4'-C5'-O5' |
| 35  | 1a    | 1402 | 4OC  | C1'-C2'-O2'-CM2 |
| 35  | 1a    | 1407 | 5MC  | O4'-C4'-C5'-O5' |
| 35  | 1a    | 1498 | UR3  | O4'-C1'-N1-C6   |
| 35  | 1a    | 1498 | UR3  | O4'-C1'-N1-C2   |
| 35  | 1a    | 1518 | MA6  | C5-C6-N6-C9     |
| 58  | 1x    | 55   | PSU  | O4'-C1'-C5-C4   |
| 58  | 1x    | 55   | PSU  | O4'-C1'-C5-C6   |
| 1   | 1A    | 1962 | 5MC  | C3'-C4'-C5'-O5' |
| 1   | 1A    | 2030 | 6MZ  | O4'-C4'-C5'-O5' |
| 1   | 1A    | 2504 | PSU  | C3'-C4'-C5'-O5' |
| 35  | 1a    | 527  | 7MG  | C3'-C4'-C5'-O5' |
| 35  | 1a    | 1207 | 2MG  | C3'-C4'-C5'-O5' |
| 35  | 1a    | 1407 | 5MC  | C3'-C4'-C5'-O5' |
| 58  | 1x    | 46   | 7MG  | O4'-C4'-C5'-O5' |
| 1   | 1A    | 746  | PSU  | C3'-C4'-C5'-O5' |
| 1   | 1A    | 1915 | 3TD  | O4'-C4'-C5'-O5' |
| 1   | 1A    | 2030 | 6MZ  | C3'-C4'-C5'-O5' |
| 1   | 1A    | 2552 | OMU  | C4'-C5'-O5'-P   |
| 35  | 1a    | 527  | 7MG  | O4'-C4'-C5'-O5' |
| 35  | 1a    | 1207 | 2MG  | O4'-C4'-C5'-O5' |
| 35  | 1a    | 527  | 7MG  | C4'-C5'-O5'-P   |
| 1   | 1A    | 2251 | OMG  | C4'-C5'-O5'-P   |
| 1   | 1A    | 2445 | 2MG  | C4'-C5'-O5'-P   |
| 35  | 1a    | 1518 | MA6  | N1-C6-N6-C9     |
| 1   | 1A    | 2552 | OMU  | O4'-C4'-C5'-O5' |
| 58  | 1x    | 46   | 7MG  | C3'-C4'-C5'-O5' |
| 1   | 1A    | 2552 | OMU  | C3'-C4'-C5'-O5' |
| 1   | 1A    | 1962 | 5MC  | C2'-C1'-N1-C6   |
| 1   | 1A    | 2457 | PSU  | O4'-C1'-C5-C4   |
| 35  | 1a    | 966  | 2MG  | C3'-C4'-C5'-O5' |
| 1   | 1A    | 2503 | 2MA  | O4'-C1'-N9-C8   |
| 1   | 1A    | 2503 | 2MA  | O4'-C1'-N9-C4   |
| 35  | 1a    | 1519 | MA6  | C5-C6-N6-C9     |
| 1   | 1A    | 747  | 5MU  | O4'-C1'-N1-C6   |
| 1   | 1A    | 2503 | 2MA  | C4'-C5'-O5'-P   |
| 35  | 1a    | 966  | 2MG  | O4'-C4'-C5'-O5' |
| 35  | 1a    | 966  | 2MG  | C4'-C5'-O5'-P   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | 1A    | 1962 | 5MC  | O4'-C1'-N1-C6   |
| 1   | 1A    | 2069 | G7M  | C4'-C5'-O5'-P   |
| 1   | 1A    | 1915 | 3TD  | O4'-C1'-C5-C6   |
| 1   | 1A    | 2457 | PSU  | O4'-C1'-C5-C6   |
| 35  | 1a    | 1402 | 4OC  | C2'-C1'-N1-C6   |
| 1   | 1A    | 2069 | G7M  | O4'-C4'-C5'-O5' |
| 1   | 1A    | 747  | 5MU  | O4'-C1'-N1-C2   |
| 35  | 1a    | 1402 | 4OC  | C2'-C1'-N1-C2   |

There are no ring outliers.

24 monomers are involved in 35 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 35  | 1a    | 1516 | 2MG  | 2       | 0            |
| 1   | 1A    | 2445 | 2MG  | 2       | 0            |
| 1   | 1A    | 1917 | PSU  | 1       | 0            |
| 1   | 1A    | 745  | 1MG  | 1       | 0            |
| 35  | 1a    | 1407 | 5MC  | 1       | 0            |
| 35  | 1a    | 1519 | MA6  | 1       | 0            |
| 1   | 1A    | 2604 | PSU  | 1       | 0            |
| 1   | 1A    | 2498 | OMC  | 1       | 0            |
| 1   | 1A    | 1835 | 2MG  | 1       | 0            |
| 1   | 1A    | 747  | 5MU  | 1       | 0            |
| 1   | 1A    | 1939 | 5MU  | 1       | 0            |
| 1   | 1A    | 1618 | 6MZ  | 1       | 0            |
| 35  | 1a    | 527  | 7MG  | 1       | 0            |
| 1   | 1A    | 2251 | OMG  | 2       | 0            |
| 1   | 1A    | 2030 | 6MZ  | 2       | 0            |
| 1   | 1A    | 1915 | 3TD  | 1       | 0            |
| 35  | 1a    | 1498 | UR3  | 3       | 0            |
| 1   | 1A    | 2069 | G7M  | 2       | 0            |
| 58  | 1x    | 46   | 7MG  | 1       | 0            |
| 35  | 1a    | 1518 | MA6  | 3       | 0            |
| 58  | 1x    | 65   | PSU  | 4       | 0            |
| 1   | 1A    | 955  | PSU  | 1       | 0            |
| 1   | 1A    | 2503 | 2MA  | 2       | 0            |
| 35  | 1a    | 1402 | 4OC  | 1       | 0            |

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

1 ligand is modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 59  | EVN  | 1A    | 3001 | 1    | 117,123,123  | 1.97 | 20 (17%)    | 155,191,191 | 1.89 | 34 (21%)    |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings      |
|-----|------|-------|------|------|---------|---------------|------------|
| 59  | EVN  | 1A    | 3001 | 1    | -       | 23/50/234/234 | 1/13/13/13 |

All (20) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 59  | 1A    | 3001 | EVN  | ODS-NDQ | 10.70 | 1.45        | 1.22     |
| 59  | 1A    | 3001 | EVN  | CDN-CAC | -6.77 | 1.38        | 1.51     |
| 59  | 1A    | 3001 | EVN  | CEG-CDI | -6.09 | 1.39        | 1.51     |
| 59  | 1A    | 3001 | EVN  | OCW-CCQ | 5.84  | 1.45        | 1.40     |
| 59  | 1A    | 3001 | EVN  | CDD-CDB | -4.60 | 1.39        | 1.50     |
| 59  | 1A    | 3001 | EVN  | CAD-CAJ | -4.36 | 1.40        | 1.50     |
| 59  | 1A    | 3001 | EVN  | ODT-CAX | 3.99  | 1.49        | 1.42     |
| 59  | 1A    | 3001 | EVN  | OCZ-CCY | 3.59  | 1.47        | 1.41     |
| 59  | 1A    | 3001 | EVN  | OCX-CCY | 3.54  | 1.47        | 1.41     |
| 59  | 1A    | 3001 | EVN  | CCT-CCS | -2.85 | 1.48        | 1.53     |
| 59  | 1A    | 3001 | EVN  | OCN-CCM | 2.64  | 1.48        | 1.43     |
| 59  | 1A    | 3001 | EVN  | OBX-CBW | 2.28  | 1.48        | 1.43     |
| 59  | 1A    | 3001 | EVN  | CAY-NDQ | -2.22 | 1.48        | 1.52     |
| 59  | 1A    | 3001 | EVN  | CBI-CBJ | -2.20 | 1.48        | 1.54     |
| 59  | 1A    | 3001 | EVN  | OBE-CBD | 2.17  | 1.43        | 1.41     |
| 59  | 1A    | 3001 | EVN  | OBK-CBD | 2.16  | 1.45        | 1.41     |
| 59  | 1A    | 3001 | EVN  | OCN-CCI | 2.15  | 1.46        | 1.41     |
| 59  | 1A    | 3001 | EVN  | OBQ-CBM | 2.09  | 1.47        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 59  | 1A    | 3001 | EVN  | OAL-CAJ | 2.07 | 1.38        | 1.34     |
| 59  | 1A    | 3001 | EVN  | CAZ-CAU | 2.03 | 1.56        | 1.51     |

All (34) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms        | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------------|-------|-------------|----------|
| 59  | 1A    | 3001 | EVN  | OCX-CCS-CCT  | -9.11 | 99.01       | 106.63   |
| 59  | 1A    | 3001 | EVN  | OCZ-CCT-CCS  | -6.12 | 98.47       | 106.41   |
| 59  | 1A    | 3001 | EVN  | CAE-CAF-CLAG | 5.99  | 128.17      | 118.95   |
| 59  | 1A    | 3001 | EVN  | OCR-CCL-CCK  | -5.49 | 94.64       | 103.54   |
| 59  | 1A    | 3001 | EVN  | CAF-CAA-CAB  | 5.05  | 123.19      | 117.78   |
| 59  | 1A    | 3001 | EVN  | O1-CCI-OCN   | 4.31  | 117.83      | 108.92   |
| 59  | 1A    | 3001 | EVN  | CAA-CAF-CAE  | -3.79 | 115.65      | 120.68   |
| 59  | 1A    | 3001 | EVN  | CAP-OAQ-CAR  | -3.48 | 104.28      | 113.82   |
| 59  | 1A    | 3001 | EVN  | CDM-ODL-CAE  | 3.47  | 124.15      | 114.74   |
| 59  | 1A    | 3001 | EVN  | CBD-OBE-CBF  | -3.38 | 109.09      | 112.16   |
| 59  | 1A    | 3001 | EVN  | CCY-OCZ-CCT  | -3.31 | 101.27      | 106.31   |
| 59  | 1A    | 3001 | EVN  | OCF-CCK-CCL  | -3.29 | 98.90       | 103.48   |
| 59  | 1A    | 3001 | EVN  | OBE-CBF-CDW  | 3.27  | 109.92      | 105.94   |
| 59  | 1A    | 3001 | EVN  | CDW-CBF-CBA  | -2.98 | 108.95      | 113.39   |
| 59  | 1A    | 3001 | EVN  | OCW-CCQ-OCR  | 2.82  | 114.32      | 109.99   |
| 59  | 1A    | 3001 | EVN  | CCM-CCL-CCK  | -2.71 | 107.47      | 112.56   |
| 59  | 1A    | 3001 | EVN  | ODL-CAE-CAD  | -2.68 | 113.95      | 120.10   |
| 59  | 1A    | 3001 | EVN  | CEF-O2-C2    | -2.65 | 107.68      | 114.47   |
| 59  | 1A    | 3001 | EVN  | CBV-O4-C4    | -2.58 | 111.85      | 117.98   |
| 59  | 1A    | 3001 | EVN  | ODJ-CDE-CDD  | -2.53 | 116.47      | 121.14   |
| 59  | 1A    | 3001 | EVN  | CAP-OAS-CBA  | -2.47 | 109.80      | 114.72   |
| 59  | 1A    | 3001 | EVN  | CAA-CAB-CAC  | -2.39 | 120.09      | 122.65   |
| 59  | 1A    | 3001 | EVN  | CDY-CBI-CBJ  | -2.32 | 108.55      | 114.82   |
| 59  | 1A    | 3001 | EVN  | OAL-CAM-CAR  | 2.31  | 112.53      | 107.82   |
| 59  | 1A    | 3001 | EVN  | OBQ-CBR-CBW  | 2.27  | 113.01      | 107.23   |
| 59  | 1A    | 3001 | EVN  | O1-C1-C2     | 2.27  | 113.50      | 109.09   |
| 59  | 1A    | 3001 | EVN  | O2-C2-C3     | -2.22 | 105.31      | 110.39   |
| 59  | 1A    | 3001 | EVN  | CDX-CBO-CBJ  | -2.17 | 109.23      | 113.55   |
| 59  | 1A    | 3001 | EVN  | O4-C4-C3     | 2.16  | 112.71      | 107.23   |
| 59  | 1A    | 3001 | EVN  | ODL-CAE-CAF  | 2.16  | 123.33      | 120.12   |
| 59  | 1A    | 3001 | EVN  | CDP-CAW-CAX  | -2.05 | 109.47      | 113.55   |
| 59  | 1A    | 3001 | EVN  | OAS-CAP-CAO  | 2.05  | 112.22      | 108.28   |
| 59  | 1A    | 3001 | EVN  | OAL-CAM-CAN  | 2.04  | 112.27      | 108.19   |
| 59  | 1A    | 3001 | EVN  | OAV-CAW-CDP  | 2.02  | 111.21      | 106.74   |

There are no chirality outliers.

All (23) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 59  | 1A    | 3001 | EVN  | C2-C1-O1-CCI    |
| 59  | 1A    | 3001 | EVN  | CAW-CAX-ODT-CDU |
| 59  | 1A    | 3001 | EVN  | OAK-CAJ-OAL-CAM |
| 59  | 1A    | 3001 | EVN  | CAD-CAJ-OAL-CAM |
| 59  | 1A    | 3001 | EVN  | CAF-CAE-ODL-CDM |
| 59  | 1A    | 3001 | EVN  | C3-C4-O4-CBV    |
| 59  | 1A    | 3001 | EVN  | CAO-CAP-OAS-CBA |
| 59  | 1A    | 3001 | EVN  | OAQ-CAP-OAS-CBA |
| 59  | 1A    | 3001 | EVN  | CAZ-CAU-OAT-CAN |
| 59  | 1A    | 3001 | EVN  | CBF-CBA-OAS-CAP |
| 59  | 1A    | 3001 | EVN  | O5-C5-C6-O6     |
| 59  | 1A    | 3001 | EVN  | CBB-CBA-OAS-CAP |
| 59  | 1A    | 3001 | EVN  | CBW-CBR-OBQ-CBM |
| 59  | 1A    | 3001 | EVN  | OAV-CAU-OAT-CAN |
| 59  | 1A    | 3001 | EVN  | CBS-CBR-OBQ-CBM |
| 59  | 1A    | 3001 | EVN  | CAD-CAE-ODL-CDM |
| 59  | 1A    | 3001 | EVN  | C5-C6-O6-CED    |
| 59  | 1A    | 3001 | EVN  | CAR-CAM-OAL-CAJ |
| 59  | 1A    | 3001 | EVN  | OCN-CCI-O1-C1   |
| 59  | 1A    | 3001 | EVN  | OBN-CBM-OBQ-CBR |
| 59  | 1A    | 3001 | EVN  | C5-C4-O4-CBV    |
| 59  | 1A    | 3001 | EVN  | CBL-CBM-OBQ-CBR |
| 59  | 1A    | 3001 | EVN  | CAZ-CAY-NDQ-ODS |

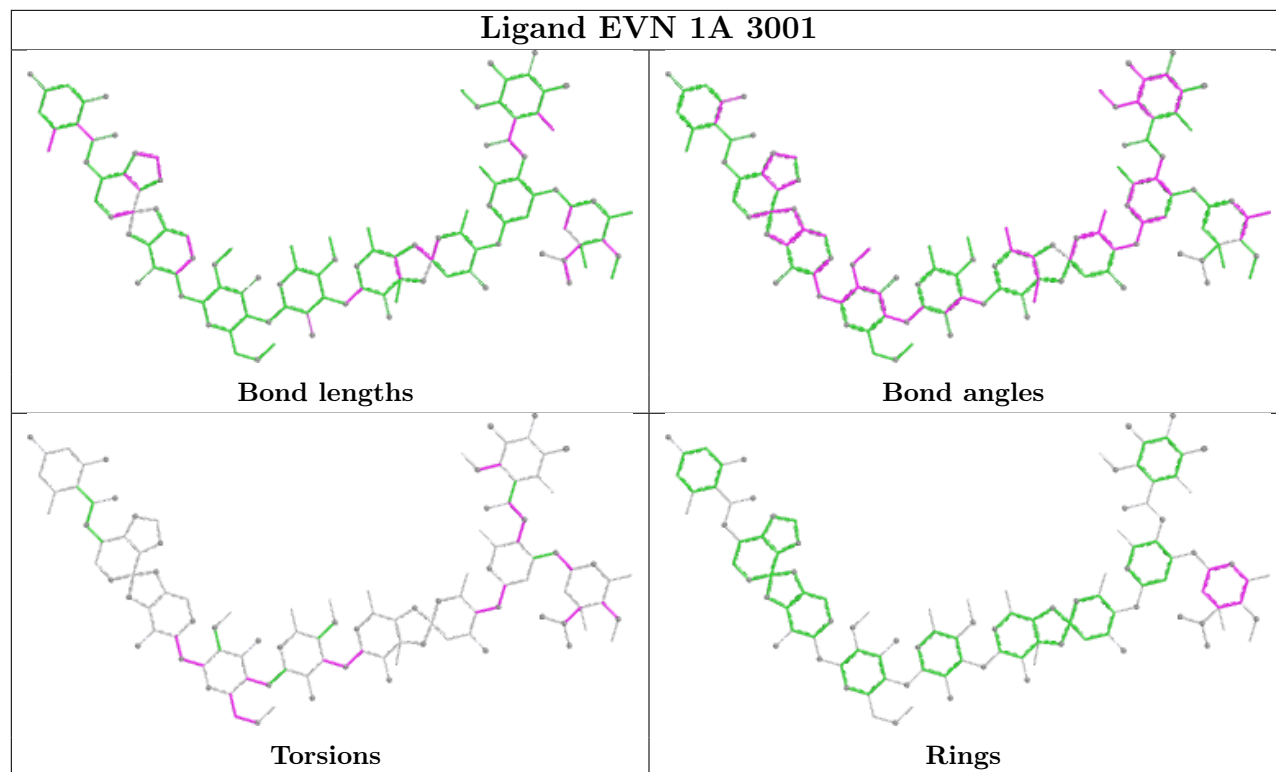
All (1) ring outliers are listed below:

| Mol | Chain | Res  | Type | Atoms                   |
|-----|-------|------|------|-------------------------|
| 59  | 1A    | 3001 | EVN  | CAU-CAW-CAX-CAY-CAZ-OAV |

No monomer is involved in short contacts.

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

equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

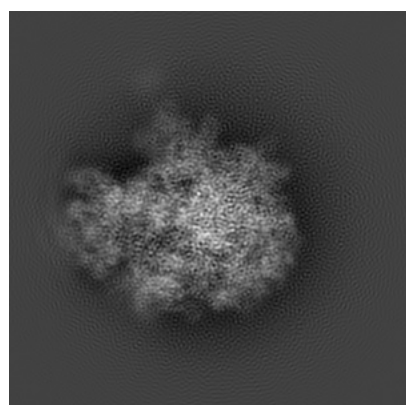
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8238. These allow visual inspection of the internal detail of the map and identification of artifacts.

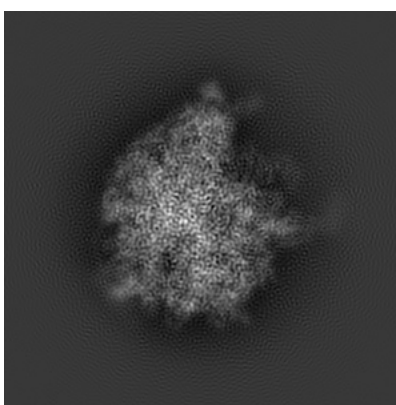
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

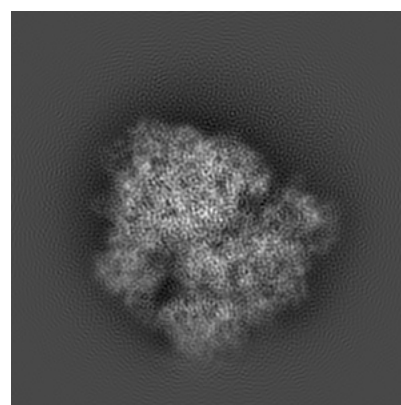
#### 6.1.1 Primary map



X



Y

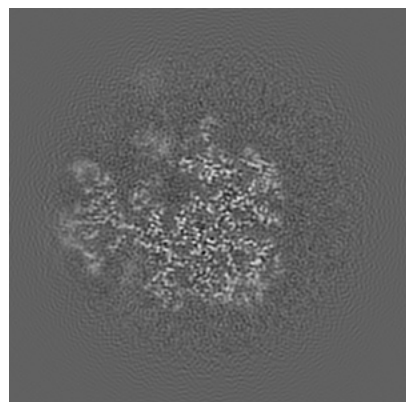


Z

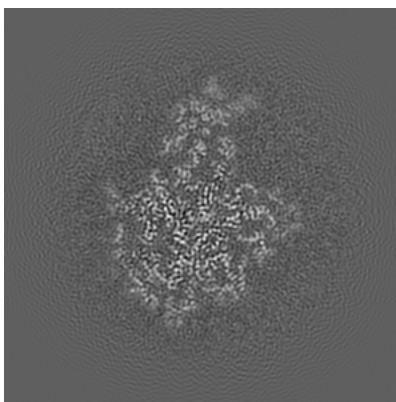
The images above show the map projected in three orthogonal directions.

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

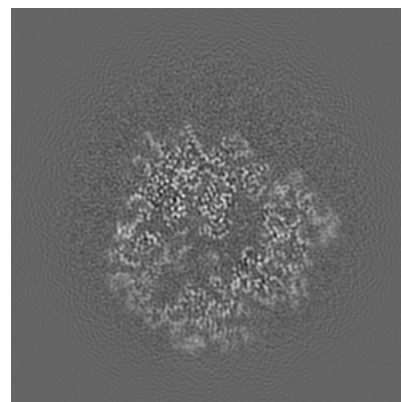
#### 6.2.1 Primary map



X Index: 184



Y Index: 184

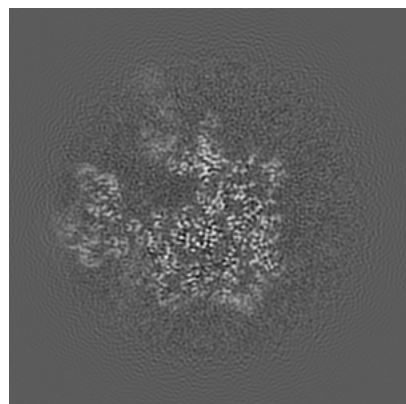


Z Index: 184

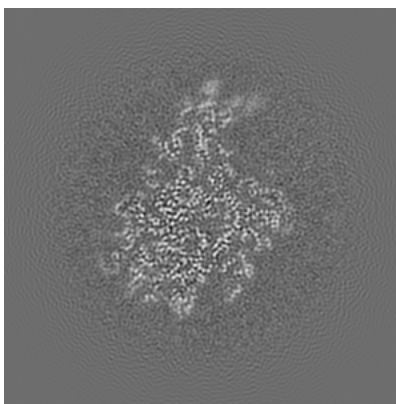
The images above show central slices of the map in three orthogonal directions.

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

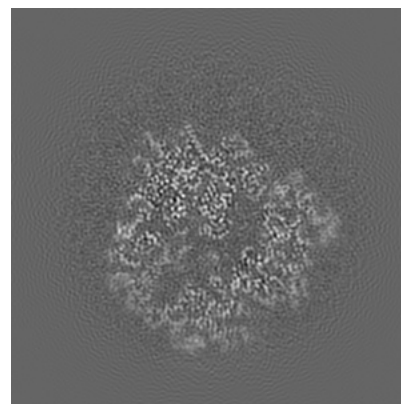
### 6.3.1 Primary map



X Index: 179



Y Index: 177

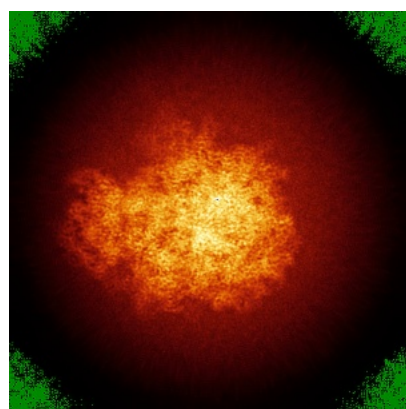


Z Index: 184

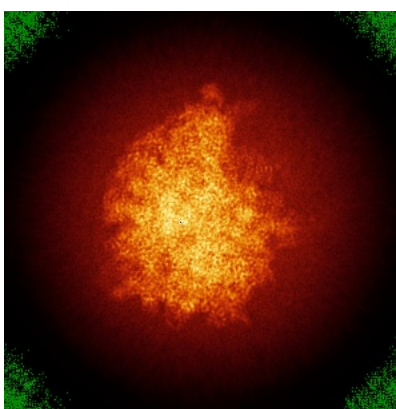
The images above show the largest variance slices of the map in three orthogonal directions.

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

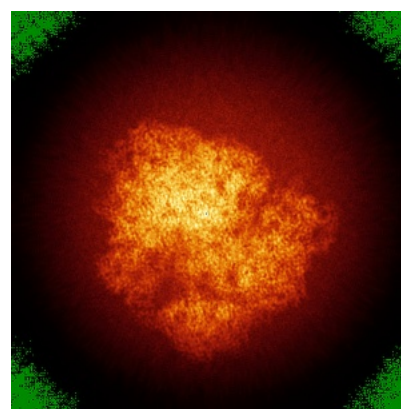
### 6.4.1 Primary map



X



Y

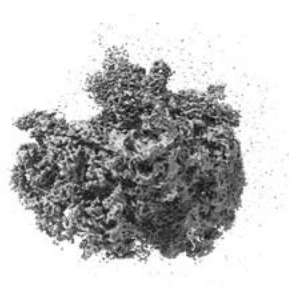


Z

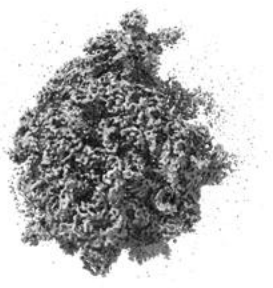
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

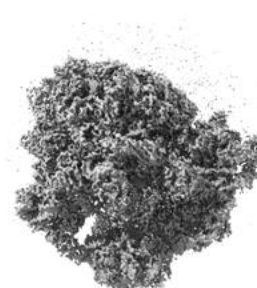
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00307. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

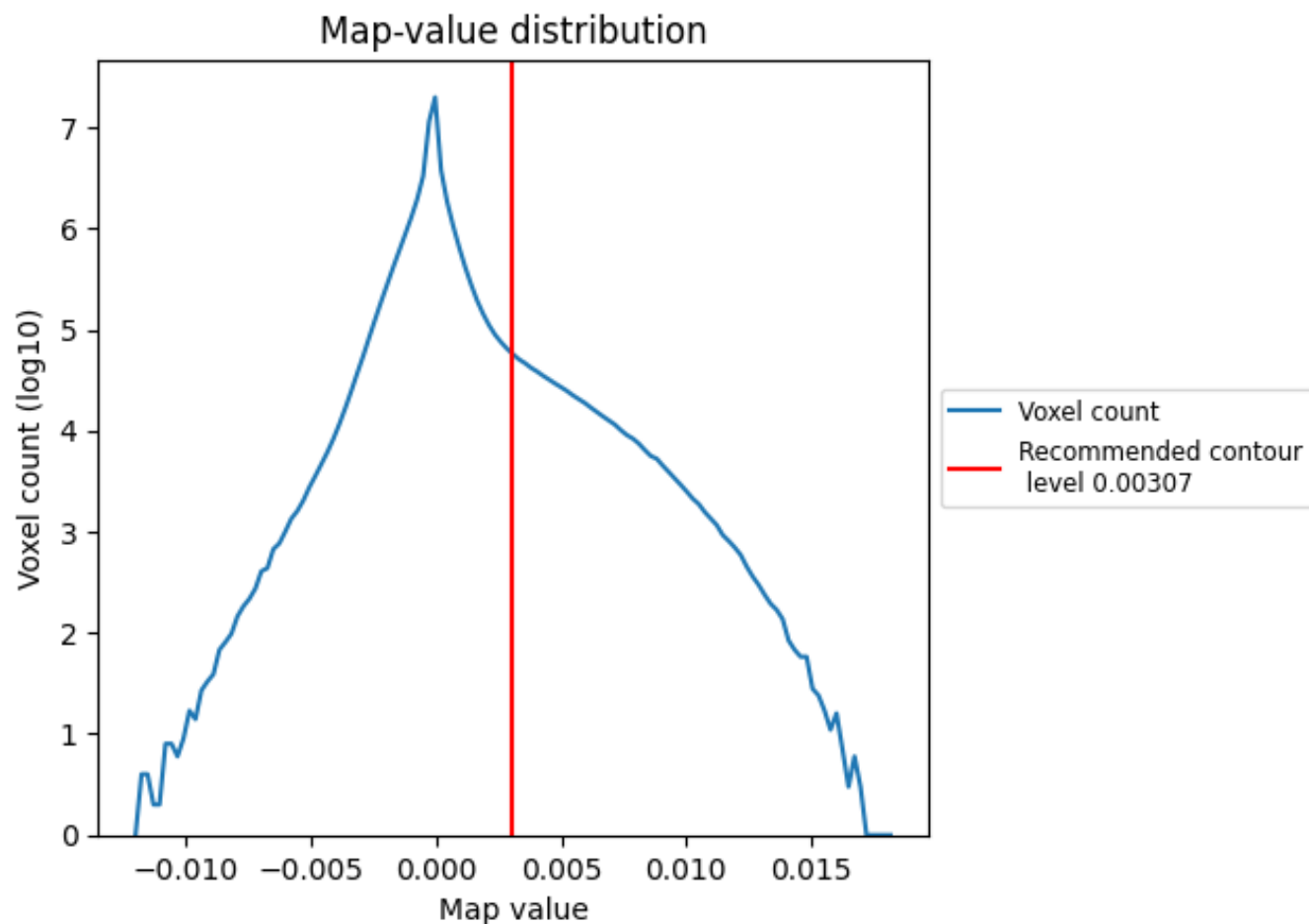
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

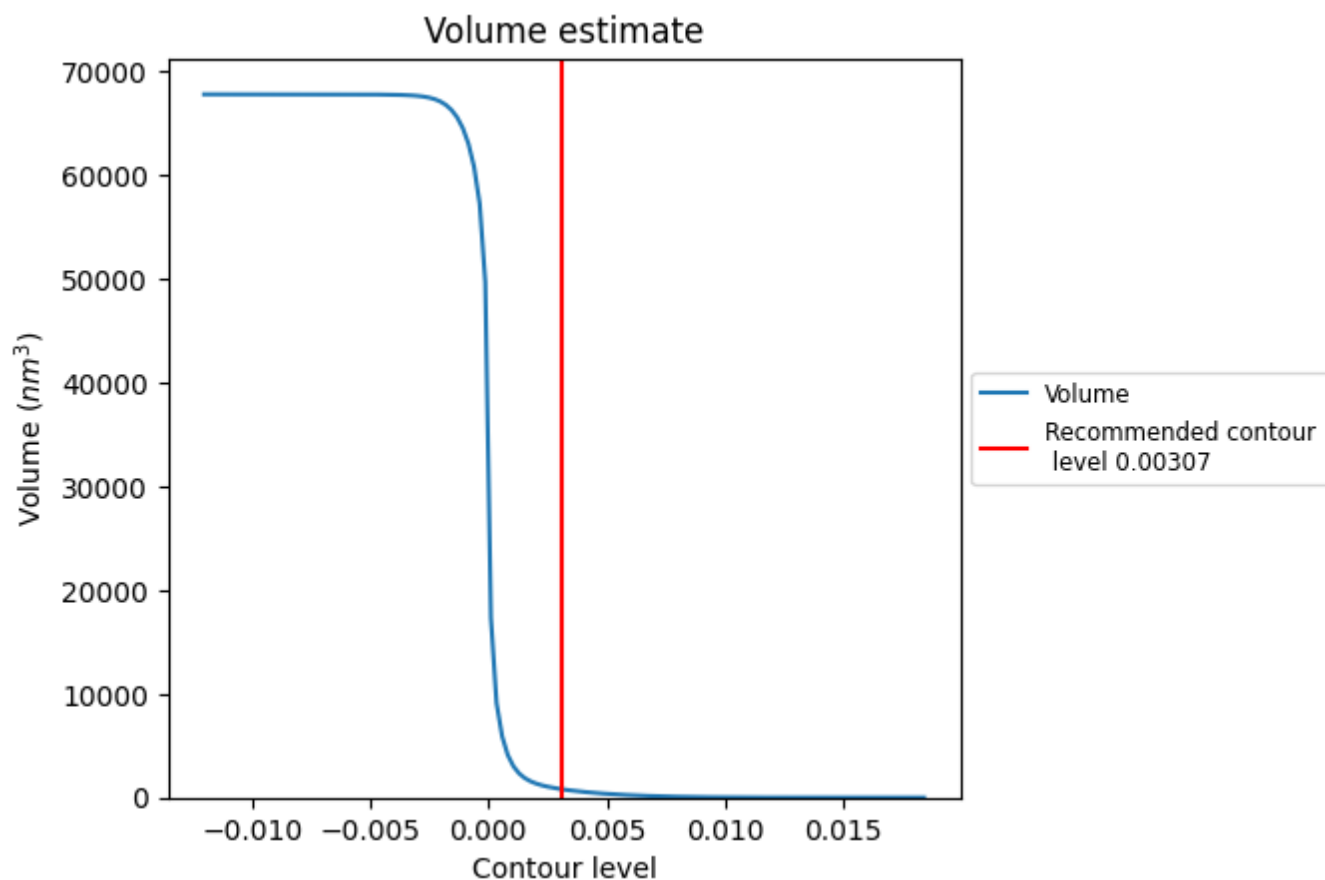
This section contains the results of statistical analysis of the map.

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



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

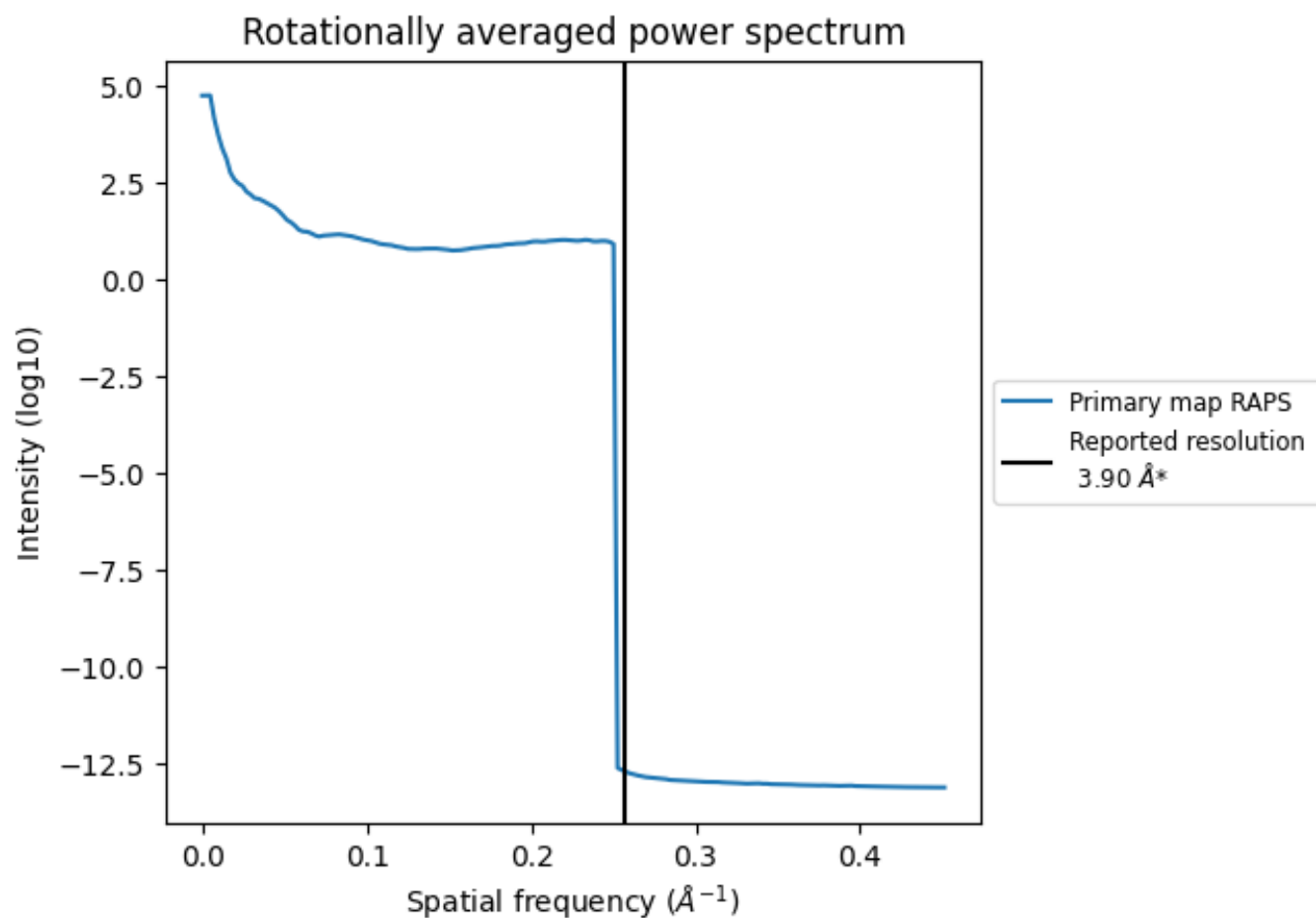
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 816 nm<sup>3</sup>; this corresponds to an approximate mass of 737 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 0.256 Å<sup>-1</sup>

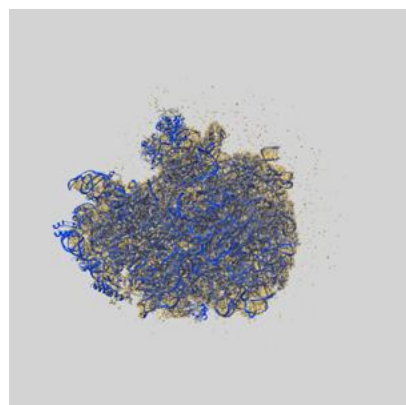
## 8 Fourier-Shell correlation

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

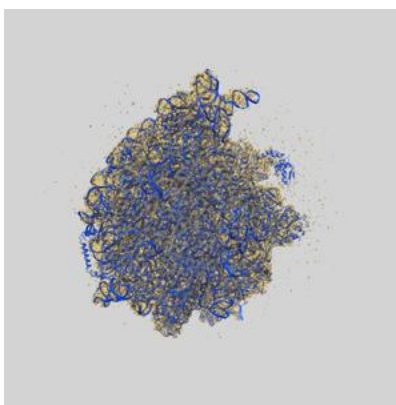
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8238 and PDB model 5KCS. Per-residue inclusion information can be found in section 3 on page 16.

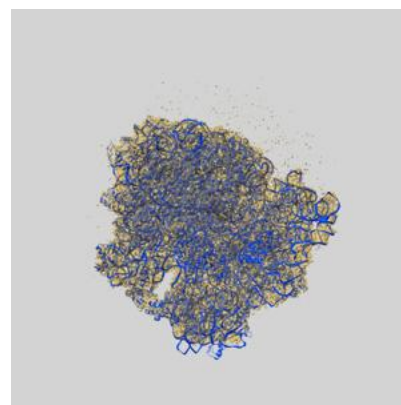
### 9.1 Map-model overlay [i](#)



X



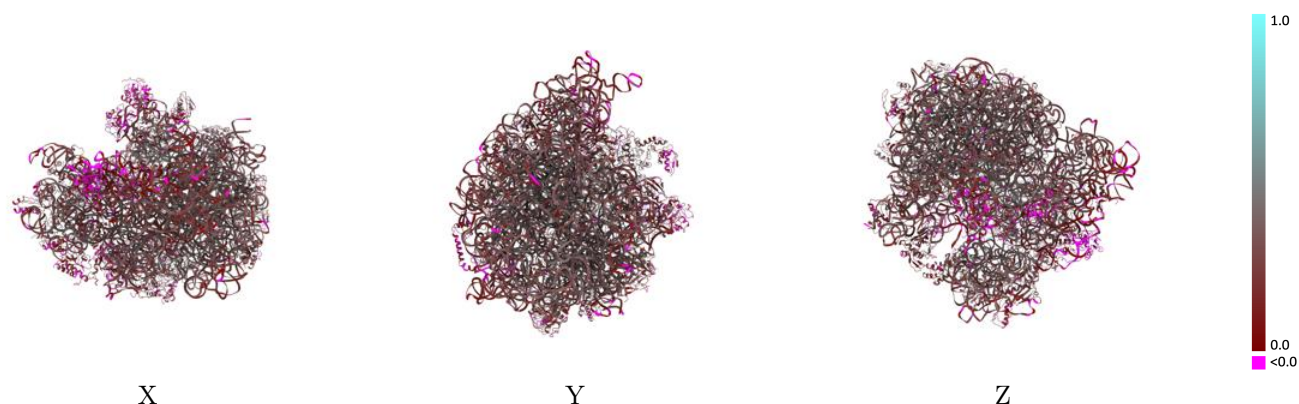
Y



Z

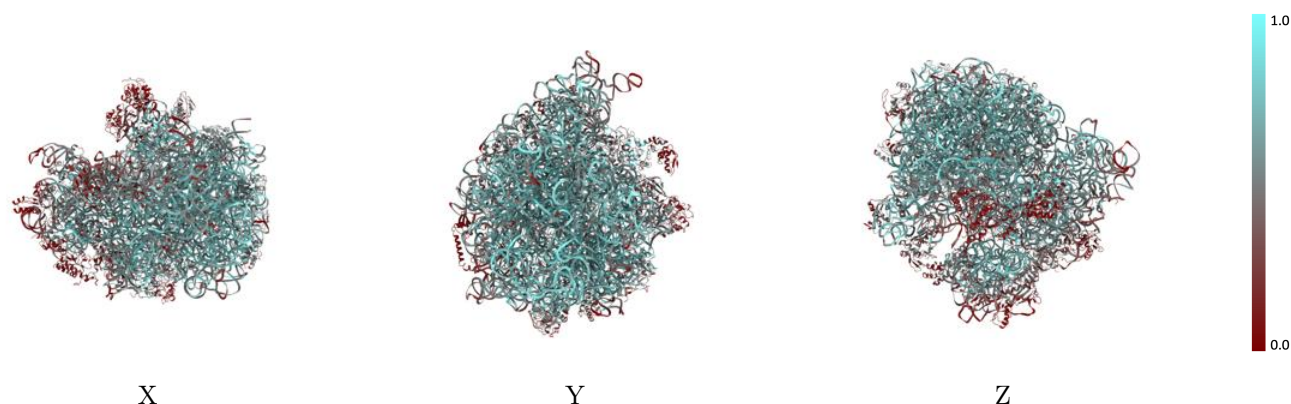
The images above show the 3D surface view of the map at the recommended contour level 0.00307 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



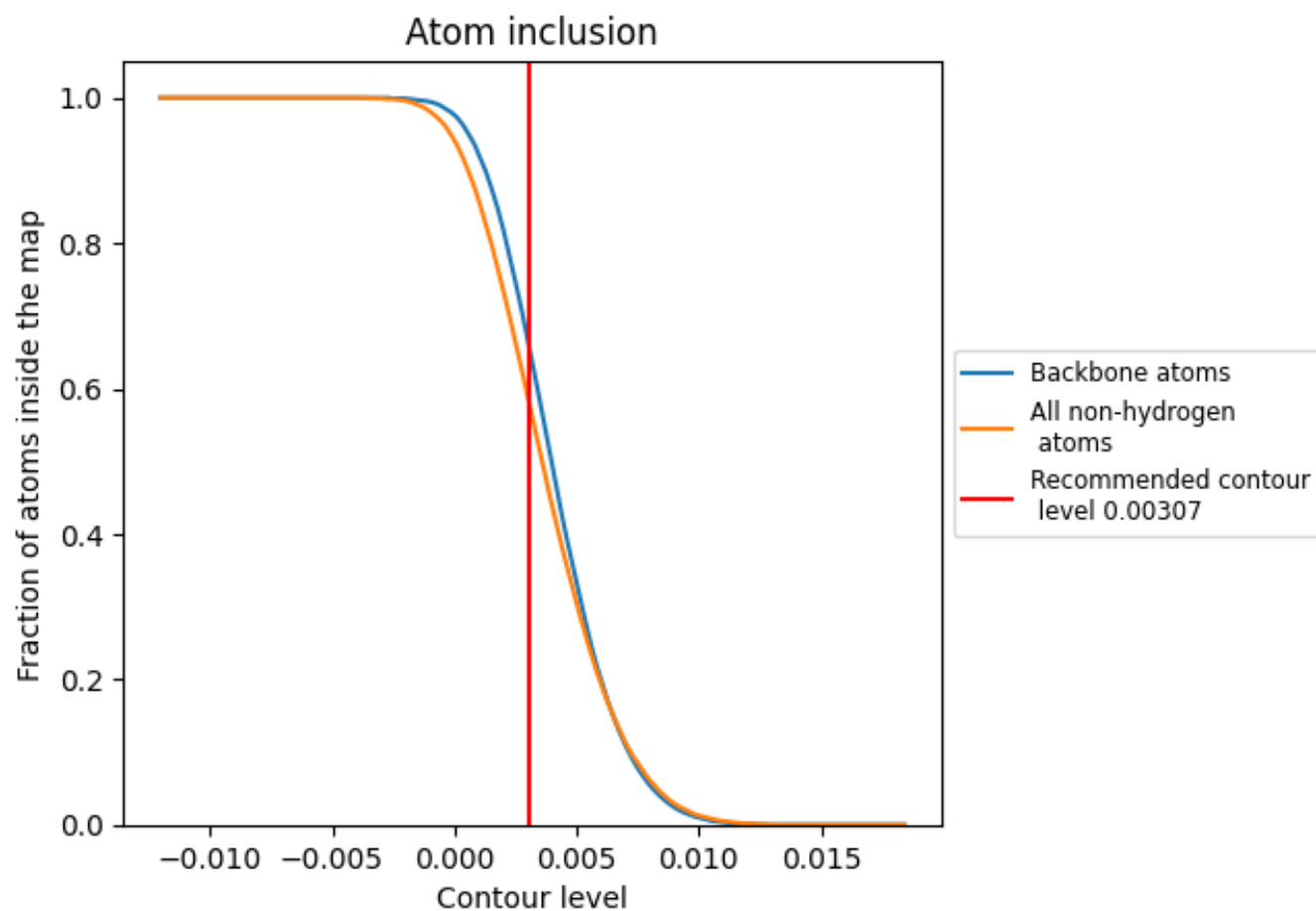
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00307).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 58% 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 (0.00307) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.5780   |  0.2930   |
| 10    |  0.5780   |  0.3400   |
| 11    |  0.5290   |  0.3340   |
| 12    |  0.4330   |  0.2550   |
| 13    |  0.5260   |  0.3310   |
| 14    |  0.2110   |  0.1720   |
| 15    |  0.5420   |  0.3270   |
| 16    |  0.0920   |  0.1900   |
| 17    |  0.6250   |  0.3430   |
| 18    |  0.5800   |  0.3540   |
| 19    |  0.5890   |  0.3360   |
| 1A    |  0.6810   |  0.3250   |
| 1B    |  0.6480   |  0.2900   |
| 1D    |  0.5860   |  0.3510   |
| 1E    |  0.5360  |  0.3240  |
| 1F    |  0.4670 |  0.2970 |
| 1G    |  0.3680 |  0.2320 |
| 1H    |  0.4030 |  0.2420 |
| 1I    |  0.0970 |  0.1240 |
| 1J    |  0.0640 |  0.0470 |
| 1K    |  0.0760 |  0.0790 |
| 1L    |  0.0510 |  0.0670 |
| 1N    |  0.5650 |  0.3080 |
| 1O    |  0.5170 |  0.3210 |
| 1P    |  0.4830 |  0.2900 |
| 1Q    |  0.5860 |  0.3890 |
| 1R    |  0.5660 |  0.3360 |
| 1S    |  0.4010 |  0.2380 |
| 1T    |  0.5100 |  0.2950 |
| 1U    |  0.6190 |  0.3520 |
| 1V    |  0.4920 |  0.2850 |
| 1W    |  0.5480 |  0.3350 |
| 1X    |  0.4830 |  0.2990 |
| 1Y    |  0.4200 |  0.2820 |
| 1Z    |  0.4730 |  0.2870 |



*Continued on next page...*

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| 1a    |  0.6150   |  0.2830   |
| 1b    |  0.1880   |  0.1630   |
| 1c    |  0.3860   |  0.2920   |
| 1d    |  0.2750   |  0.0620   |
| 1e    |  0.4270   |  0.2330   |
| 1f    |  0.4120   |  0.2290   |
| 1g    |  0.3210   |  0.2650   |
| 1h    |  0.4760   |  0.2870   |
| 1i    |  0.2630   |  0.2500   |
| 1j    |  0.2180   |  0.2390   |
| 1k    |  0.3800   |  0.1990   |
| 1l    |  0.3050   |  0.0930   |
| 1m    |  0.3770   |  0.2740   |
| 1n    |  0.4360   |  0.3030   |
| 1o    |  0.4940   |  0.2860   |
| 1p    |  0.4240   |  0.1710   |
| 1q    |  0.4210   |  0.2330   |
| 1r    |  0.4890   |  0.3050   |
| 1s    |  0.4410   |  0.2780   |
| 1t    |  0.4520  |  0.2520  |
| 1u    |  0.1510 |  0.1390 |
| 1v    |  0.4640 |  0.2870 |
| 1w    |  0.5510 |  0.3290 |
| 1x    |  0.5840 |  0.3020 |