



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:38 PM UTC

PDB ID : 7K54 / pdb\_00007k54  
EMDB ID : EMD-22673  
Title : Mid-translocated +1-frameshifting(CCC-A) complex with EF-G and GDPCP (Structure II-FS)  
Authors : Demo, G.; Loveland, A.B.; Svidritskiy, E.; Gamper, H.B.; Hou, Y.M.; Korostelev, A.A.  
Deposited on : 2020-09-16  
Resolution : 3.20 Å(reported)  
Based on initial models : 6ENJ, 5UYM, 4V9P, 4V7D

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:

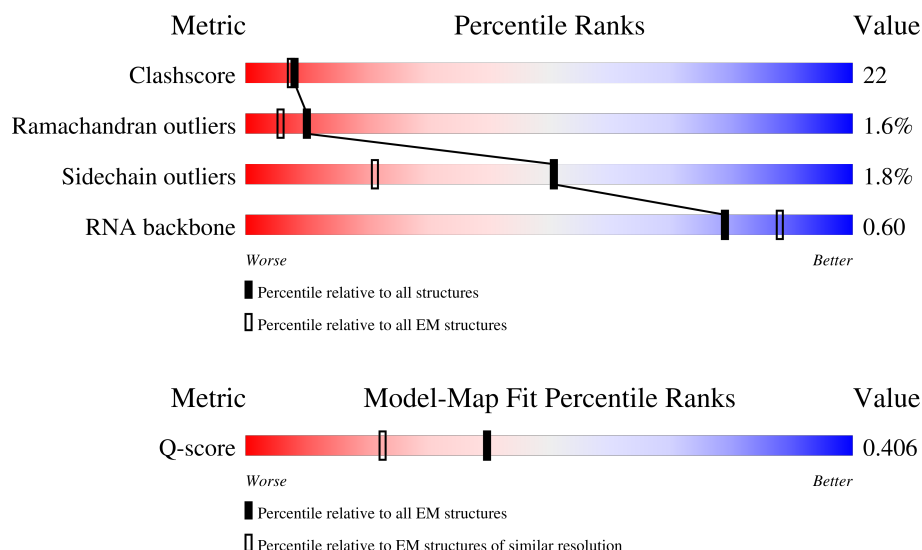
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.20 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                       | 15020 ( 2.70 - 3.70 )                                    |

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   | b     | 271    |                  |
| 2   | c     | 209    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | d     | 201    |                  |
| 4   | e     | 177    |                  |
| 5   | f     | 176    |                  |
| 6   | g     | 149    |                  |
| 7   | h     | 131    |                  |
| 8   | i     | 141    |                  |
| 9   | j     | 142    |                  |
| 10  | k     | 122    |                  |
| 11  | l     | 143    |                  |
| 12  | m     | 136    |                  |
| 13  | n     | 120    |                  |
| 14  | o     | 116    |                  |
| 15  | p     | 114    |                  |
| 16  | q     | 117    |                  |
| 17  | r     | 103    |                  |
| 18  | s     | 110    |                  |
| 19  | t     | 93     |                  |
| 20  | u     | 102    |                  |
| 21  | v     | 94     |                  |
| 22  | w     | 75     |                  |
| 23  | x     | 77     |                  |
| 24  | y     | 63     |                  |
| 25  | z     | 58     |                  |
| 26  | A     | 66     |                  |
| 27  | B     | 56     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | C     | 50     |                  |
| 29  | D     | 46     |                  |
| 30  | E     | 64     |                  |
| 31  | F     | 38     |                  |
| 32  | G     | 225    |                  |
| 33  | H     | 206    |                  |
| 34  | I     | 205    |                  |
| 35  | J     | 157    |                  |
| 36  | K     | 100    |                  |
| 37  | L     | 151    |                  |
| 38  | M     | 129    |                  |
| 39  | N     | 127    |                  |
| 40  | O     | 98     |                  |
| 41  | P     | 116    |                  |
| 42  | Q     | 123    |                  |
| 43  | R     | 114    |                  |
| 44  | S     | 100    |                  |
| 45  | T     | 88     |                  |
| 46  | U     | 82     |                  |
| 47  | V     | 80     |                  |
| 48  | W     | 65     |                  |
| 49  | X     | 79     |                  |
| 50  | Y     | 85     |                  |
| 51  | Z     | 65     |                  |
| 52  | a     | 223    |                  |

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| Mol | Chain | Length | Quality of chain                                                                        |
|-----|-------|--------|-----------------------------------------------------------------------------------------|
| 53  | 3     | 1539   | <div><div><div></div><div></div><div></div></div><div>37%51%10%</div><div></div></div>  |
| 54  | 1     | 2903   | <div><div><div></div><div></div><div></div></div><div>45%47%8%</div><div></div></div>   |
| 55  | 2     | 120    | <div><div><div></div><div></div><div></div></div><div>48%42%8%</div><div></div></div>   |
| 56  | 5     | 77     | <div><div><div></div><div></div><div></div></div><div>36%51%10%</div><div></div></div>  |
| 57  | 6     | 77     | <div><div><div></div><div></div><div></div></div><div>48%39%13%</div><div></div></div>  |
| 58  | 4     | 16     | <div><div><div></div><div></div><div></div></div><div>31%62%6%</div><div></div></div>   |
| 59  | 8     | 711    | <div><div><div></div><div></div><div></div></div><div>6%35%51%9%</div><div></div></div> |

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 153368 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | b     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2083  | 1288 | 423 | 365 | 7 |         |       |

- Molecule 2 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | c     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | d     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | e     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1411  | 899 | 249 | 257 | 6 |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | f     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | g     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 936   | 590 | 166 | 179 | 1 |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | h     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 633   | 397 | 114 | 118 | 4 |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | i     | 74       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 551   | 358 | 91 | 99 | 3 |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | j     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | k     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 939   | 587 | 180 | 166 | 6 |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | l     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | m     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | n     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 961   | 593 | 196 | 167 | 5 |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 14  | o     | 116      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 15  | p     | 114      | Total | C   | N   | O   | S       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1       | 0     |

- Molecule 16 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 16  | q     | 117      | Total | C   | N   | O   |         | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         | 0     |

- Molecule 17 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 17  | r     | 103      | Total | C   | N   | O   | S       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2       | 0     |

- Molecule 18 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 18  | s     | 110      | Total | C   | N   | O   | S       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3       | 0     |

- Molecule 19 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 19  | t     | 93       | Total | C   | N   | O   | S       | 0     |
|     |       |          | 739   | 466 | 139 | 132 | 2       | 0     |

- Molecule 20 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 20  | u     | 102      | Total | C   | N   | O   |         | 0     |
|     |       |          | 780   | 492 | 146 | 142 |         | 0     |

- Molecule 21 is a protein called 50S ribosomal protein L25.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | v     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | w     | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 575   | 356 | 116 | 102 | 1 |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | x     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 24  | y     | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 25  | z     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | A     | 66       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 523   | 323 | 99 | 95 | 6 |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 28  | C     | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 410   | 263 | 75 | 72 |         |       |

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

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

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

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

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

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

- Molecule 32 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 32  | G     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1705  | 1081 | 305 | 312 | 7 |         |       |

- Molecule 33 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 33  | H     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1625  | 1028 | 305 | 289 | 3 |         |       |

- Molecule 34 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34  | I     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 35 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | J     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1157  | 719 | 218 | 214 | 6 |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | K     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 818   | 515 | 148 | 149 | 6 |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | L     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1182  | 735 | 227 | 216 | 4 |         |       |

- Molecule 38 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | M     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 39 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | N     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | O     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 787   | 493 | 150 | 143 | 1 |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | P     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 870   | 535 | 173 | 159 | 3 |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | Q     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | R     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 884   | 546 | 178 | 157 | 3 |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | S     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 45 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | T     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 46 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | U     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | V     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 411 | 121 | 114 | 3 |         |       |

- Molecule 48 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 48  | W     | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 536   | 339 | 100 | 96 | 1 |         |       |

- Molecule 49 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | X     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 638   | 408 | 120 | 108 | 2 |         |       |

- Molecule 50 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | Y     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |       |

- Molecule 51 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 51  | Z     | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 545   | 335 | 117 | 92 | 1 |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | a     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1027  | 645 | 186 | 194 | 2 |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 54  | 1     | 2903     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62317 | 27801 | 11468 | 20146 | 2902 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference    |
|-------|---------|----------|--------|----------|--------------|
| 1     | 747     | C        | U      | conflict | GB 802133627 |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 55  | 2     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2568  | 1145 | 471 | 833 | 119 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference     |
|-------|---------|----------|--------|-----------|---------------|
| 2     | 120     | A        | -      | insertion | GB 1266961702 |

- Molecule 56 is a RNA chain called tRNAPro.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 56  | 5     | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1647  | 733 | 295 | 542 | 77 |         |       |

- Molecule 57 is a RNA chain called tRNAfMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 57  | 6     | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |       |

- Molecule 58 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 58  | 4     | 16       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 346   | 155 | 68 | 107 | 16 |         |       |

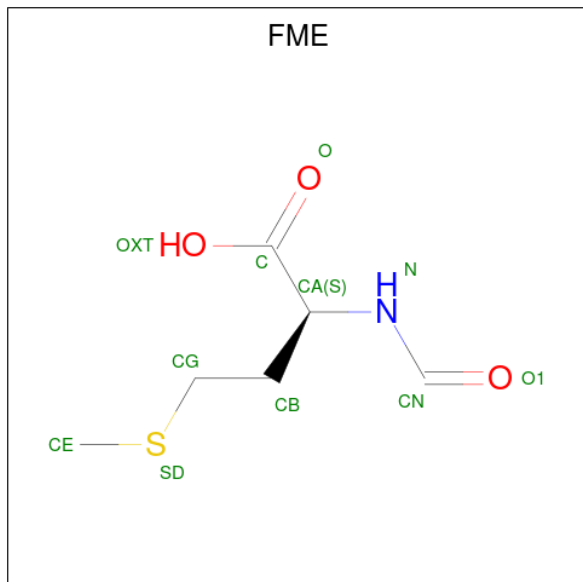
- Molecule 59 is a protein called Elongation factor G.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 59  | 8     | 685      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5312  | 3351 | 911 | 1025 | 25 |         |       |

There are 8 discrepancies between the modelled and reference sequences:

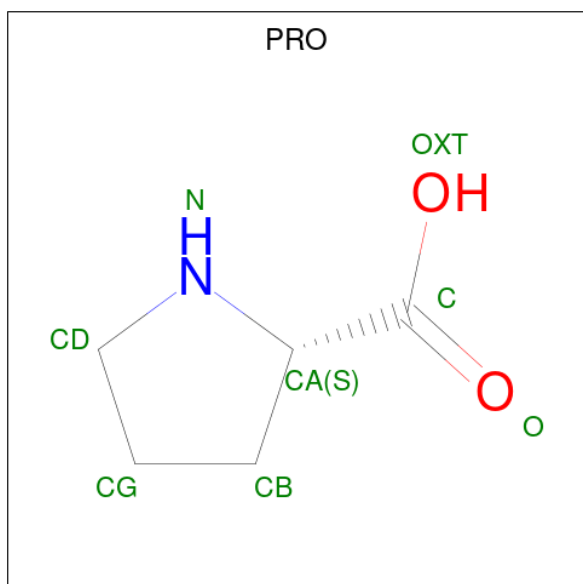
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| 8     | 705     | LEU      | -      | expression tag | UNP U9XYS4 |
| 8     | 706     | GLU      | -      | expression tag | UNP U9XYS4 |
| 8     | 707     | HIS      | -      | expression tag | UNP U9XYS4 |
| 8     | 708     | HIS      | -      | expression tag | UNP U9XYS4 |
| 8     | 709     | HIS      | -      | expression tag | UNP U9XYS4 |
| 8     | 710     | HIS      | -      | expression tag | UNP U9XYS4 |
| 8     | 711     | HIS      | -      | expression tag | UNP U9XYS4 |
| 8     | 712     | HIS      | -      | expression tag | UNP U9XYS4 |

- Molecule 60 is N-FORMYLMETHIONINE (CCD ID: FME) (formula:  $C_6H_{11}NO_3S$ ) (labeled as "Ligand of Interest" by depositor).



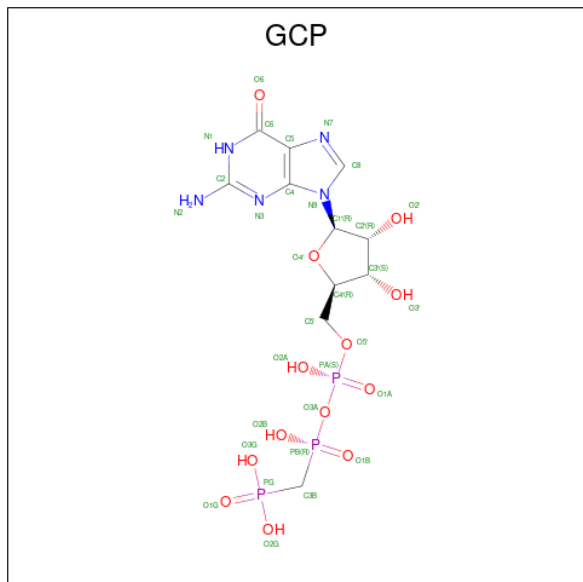
| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
|     |       |          | Total | C | N | O | S |         |
| 60  | 1     | 1        | 10    | 6 | 1 | 2 | 1 | 0       |

- Molecule 61 is PROLINE (CCD ID: PRO) (formula:  $C_5H_9NO_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
|     |       |          | Total | C | N | O |         |
| 61  | 5     | 1        | 7     | 5 | 1 | 1 | 0       |

- Molecule 62 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 62  | 8     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 11 | 5 | 13 | 3 |         |

- Molecule 63 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

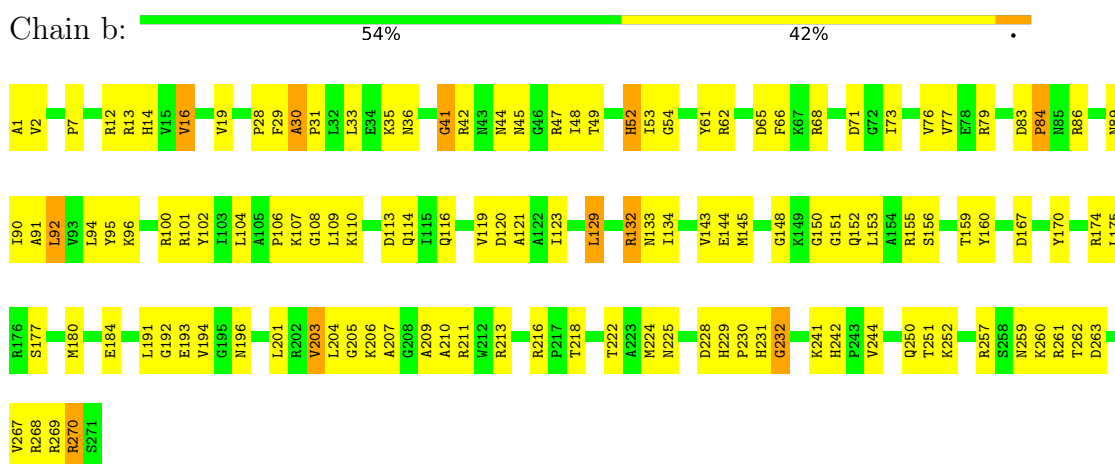
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 63  | 8     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |



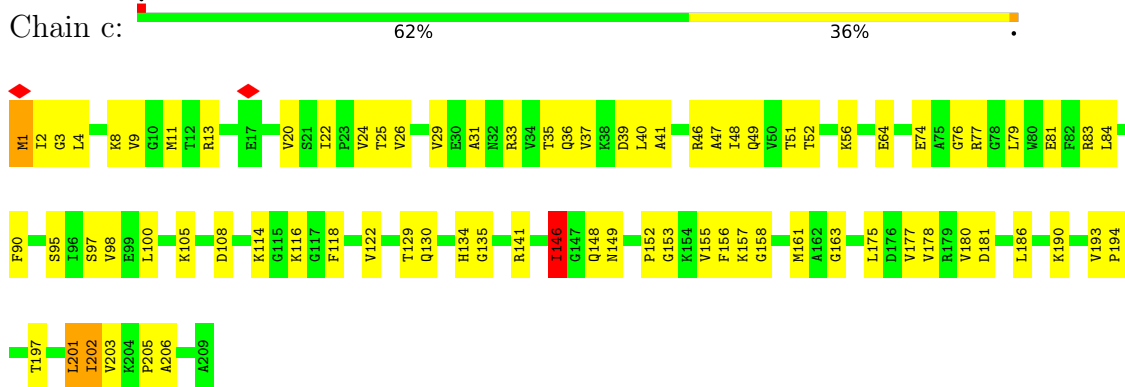
### 3 Residue-property plots

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

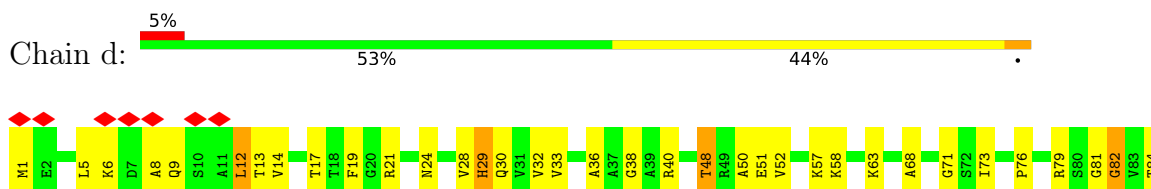
#### • Molecule 1: 50S ribosomal protein L2

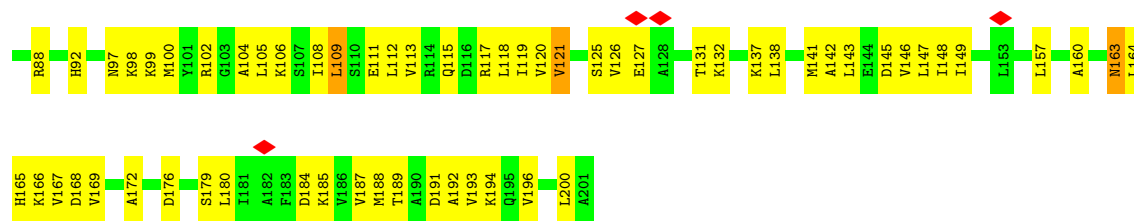


#### • Molecule 2: 50S ribosomal protein L3



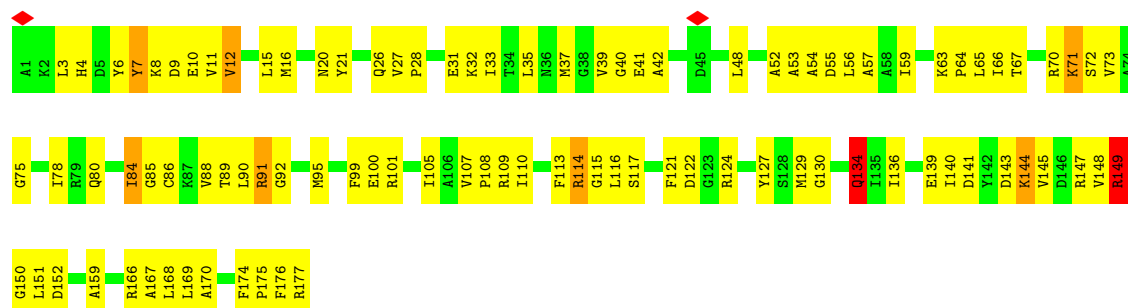
#### • Molecule 3: 50S ribosomal protein L4





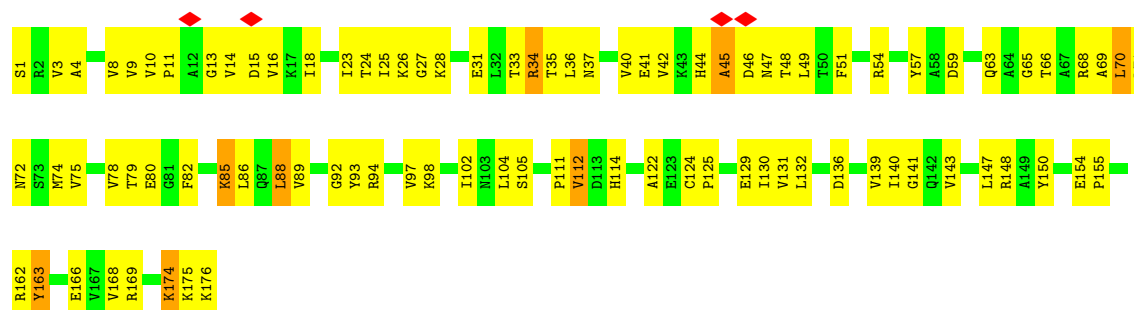
• Molecule 4: 50S ribosomal protein L5

Chain e: 45% 50% . .



• Molecule 5: 50S ribosomal protein L6

Chain f: 48% 47% 5%

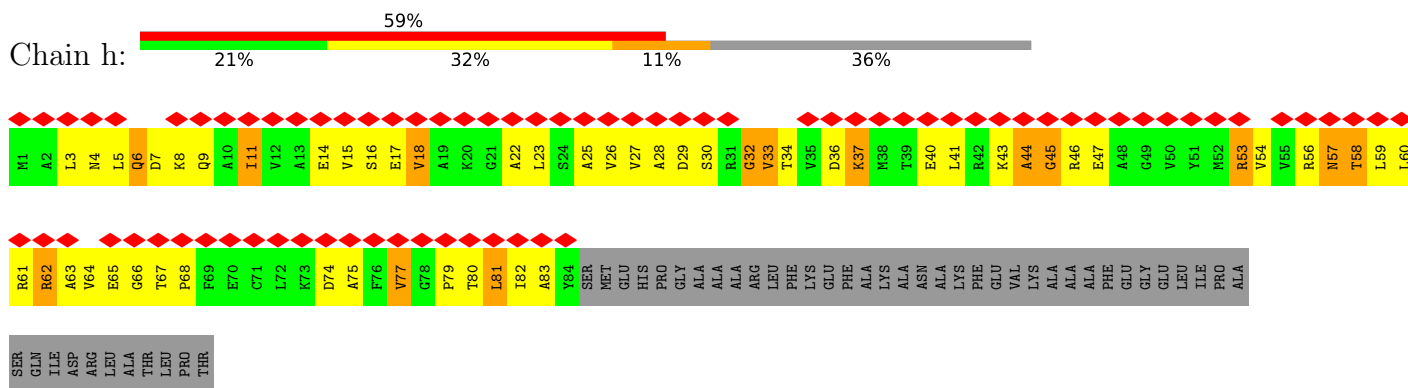


• Molecule 6: 50S ribosomal protein L9

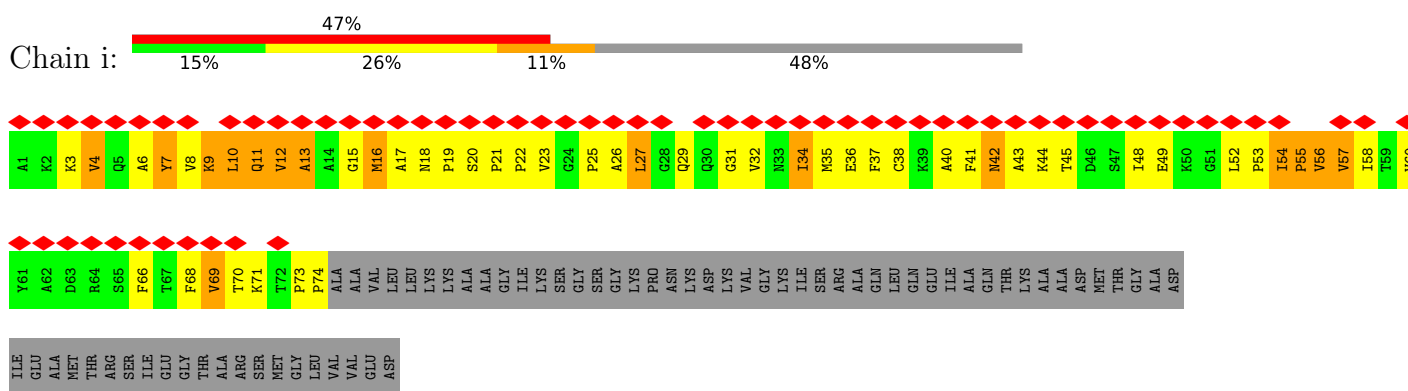
Chain g: 58% 42% 33% 8% 16%



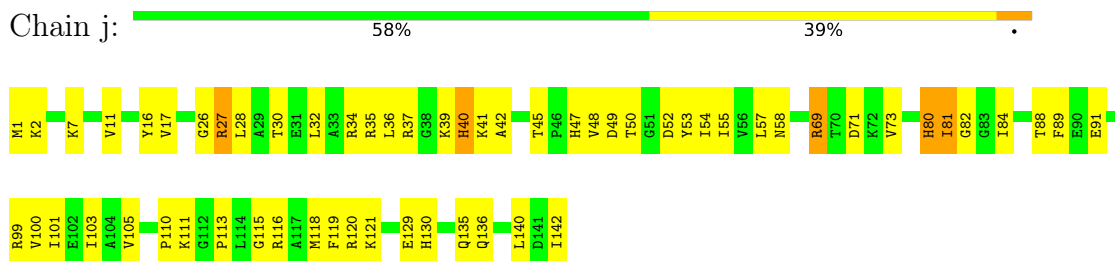
- Molecule 7: 50S ribosomal protein L10



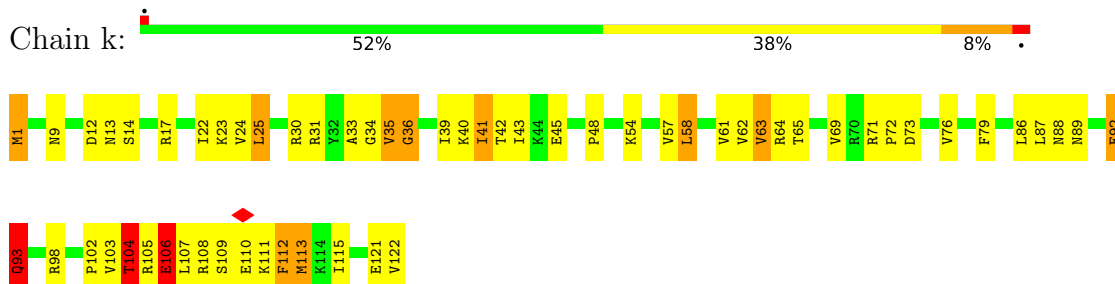
- Molecule 8: 50S ribosomal protein L11



- Molecule 9: 50S ribosomal protein L13

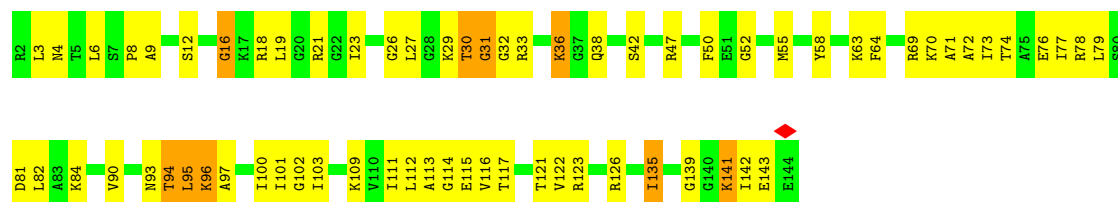


- Molecule 10: 50S ribosomal protein L14

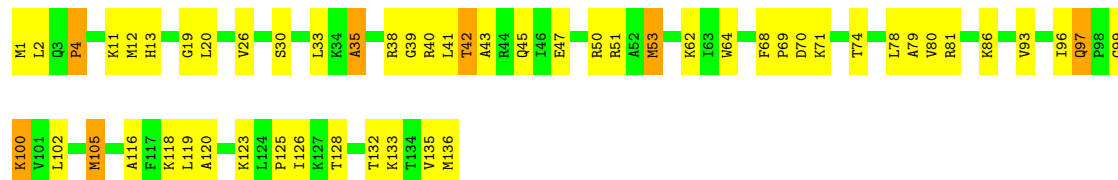


- Molecule 11: 50S ribosomal protein L15

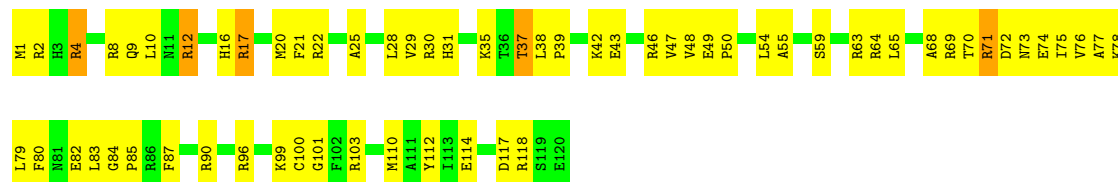




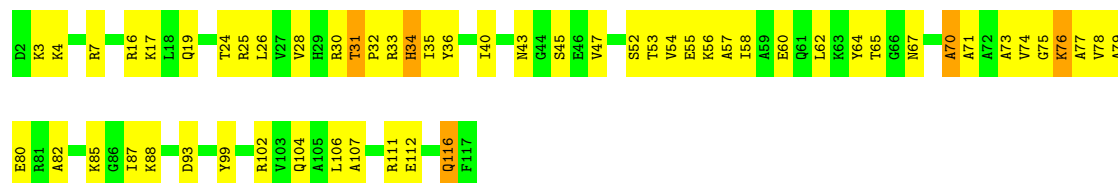
• Molecule 12: 50S ribosomal protein L16



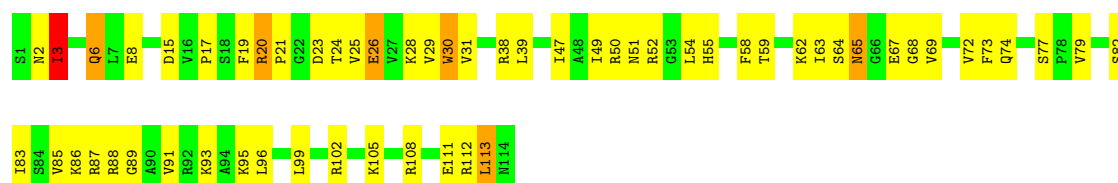
• Molecule 13: 50S ribosomal protein L17



• Molecule 14: 50S ribosomal protein L18

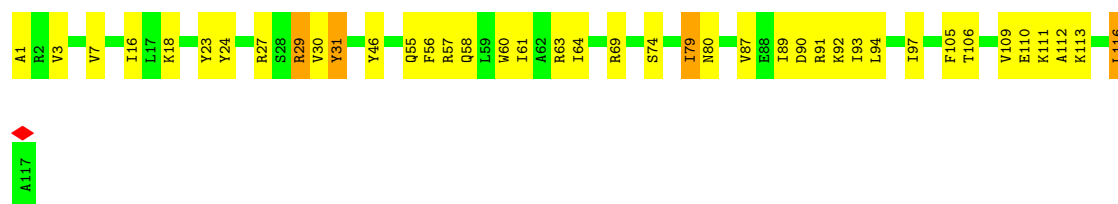


• Molecule 15: 50S ribosomal protein L19



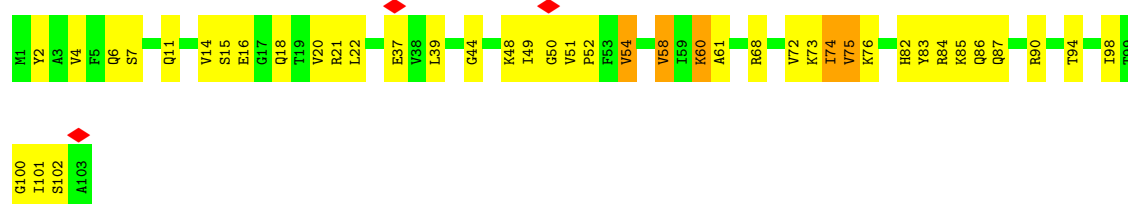
• Molecule 16: 50S ribosomal protein L20

Chain q: 



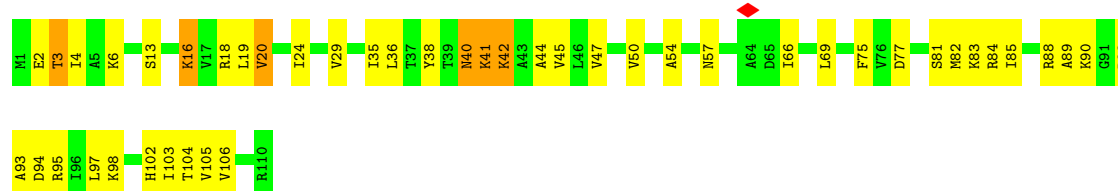
- Molecule 17: 50S ribosomal protein L21

Chain r: 



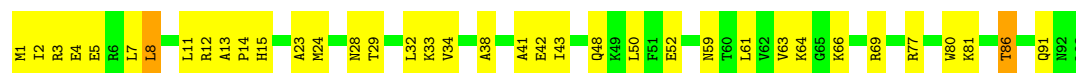
- Molecule 18: 50S ribosomal protein L22

Chain s: 



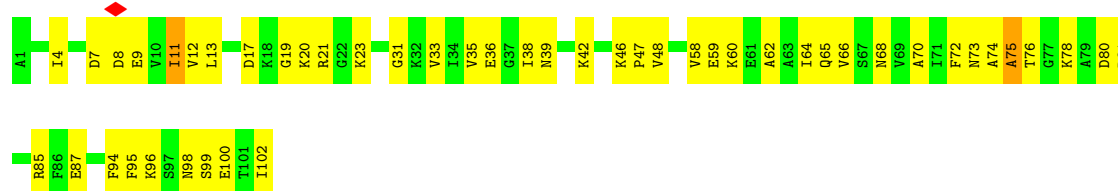
- Molecule 19: 50S ribosomal protein L23

Chain t: 



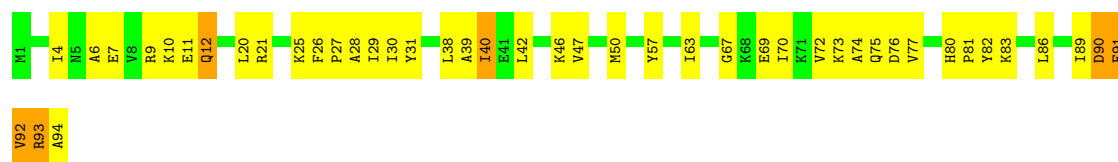
- Molecule 20: 50S ribosomal protein L24

Chain u: 



- Molecule 21: 50S ribosomal protein L25

Chain v: 



- Molecule 22: 50S ribosomal protein L27

Chain w: 



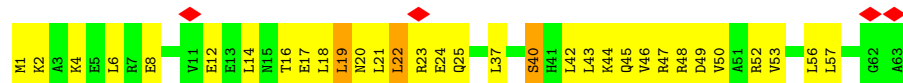
- Molecule 23: 50S ribosomal protein L28

Chain x: 



- Molecule 24: 50S ribosomal protein L29

Chain y: 



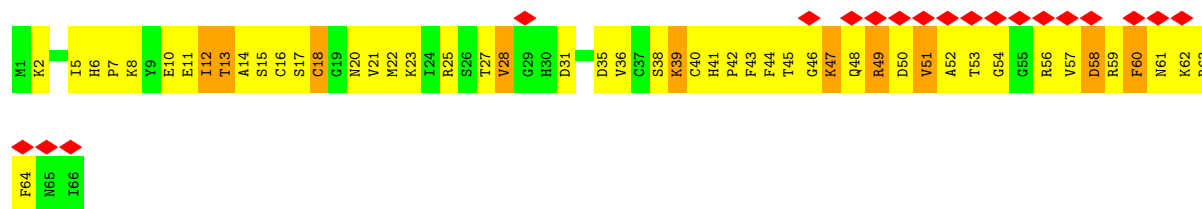
- Molecule 25: 50S ribosomal protein L30

Chain z: 



- Molecule 26: 50S ribosomal protein L31

Chain A: 



- Molecule 27: 50S ribosomal protein L32

Chain B:  59% 41%



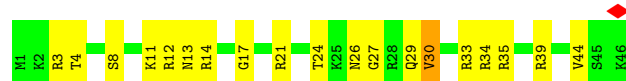
- Molecule 28: 50S ribosomal protein L33

Chain C:  6% 66% 26% 8%



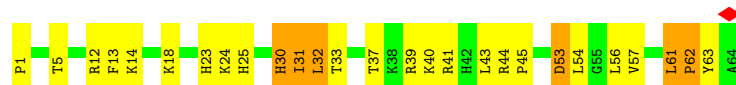
- Molecule 29: 50S ribosomal protein L34

Chain D:  59% 39%



- Molecule 30: 50S ribosomal protein L35

Chain E:  58% 33% 9%



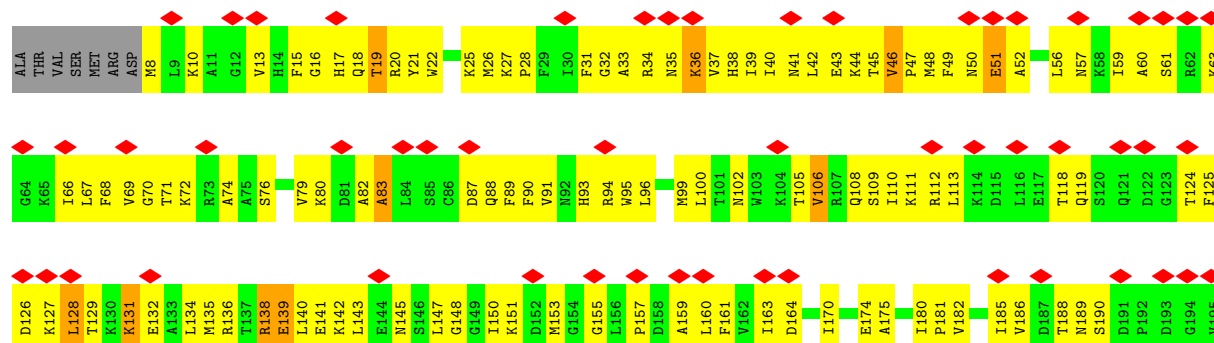
- Molecule 31: 50S ribosomal protein L36

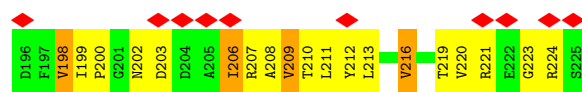
Chain F:  50% 47%



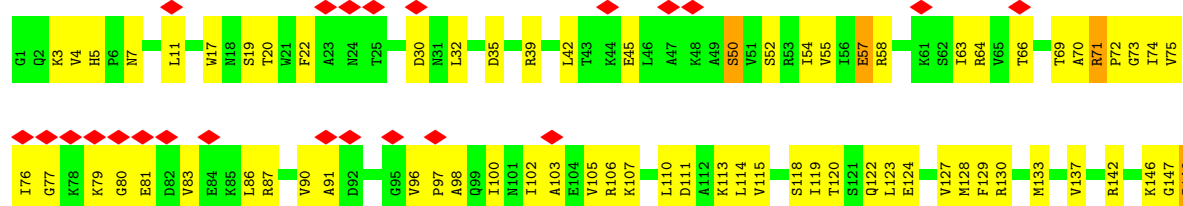
- Molecule 32: 30S ribosomal protein S2

Chain G:  28% 36% 55% 6%

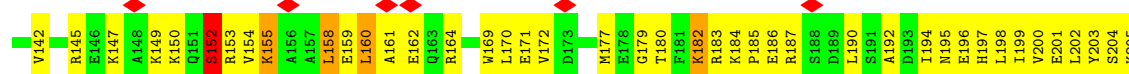




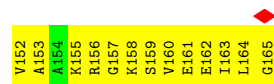
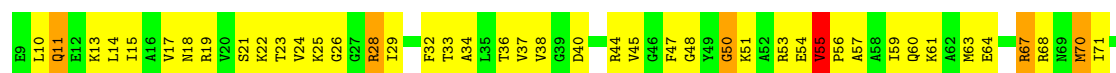
• Molecule 33: 30S ribosomal protein S3



• Molecule 34: 30S ribosomal protein S4



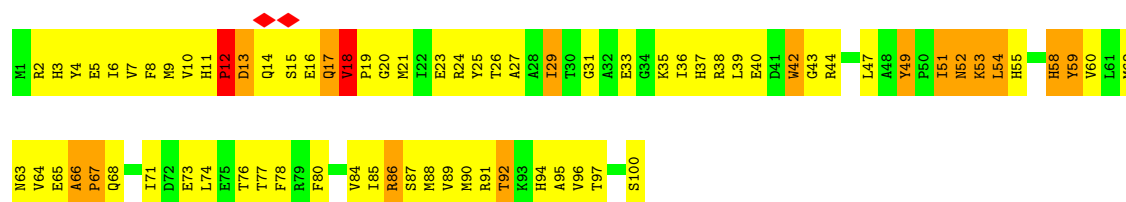
• Molecule 35: 30S ribosomal protein S5



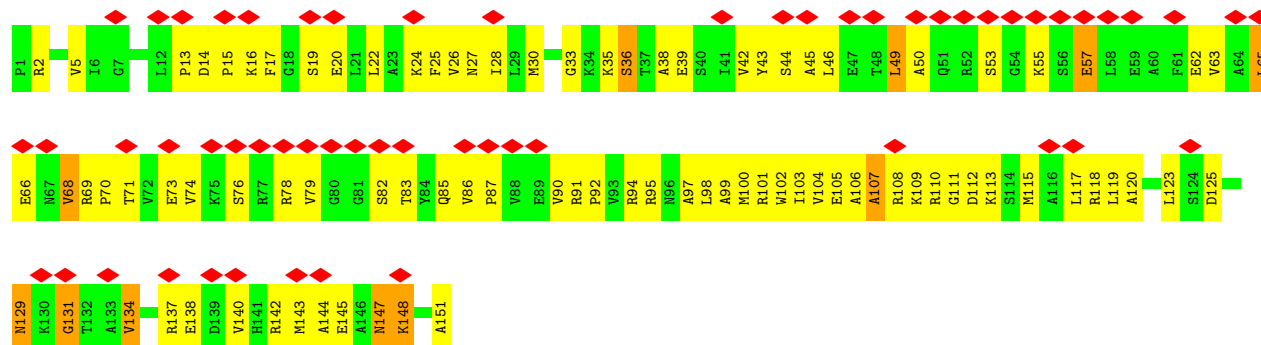
• Molecule 36: 30S ribosomal protein S6



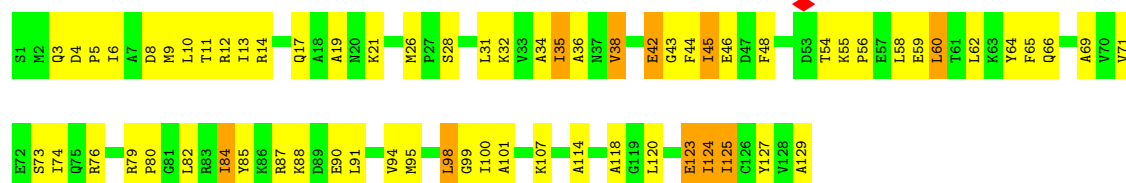




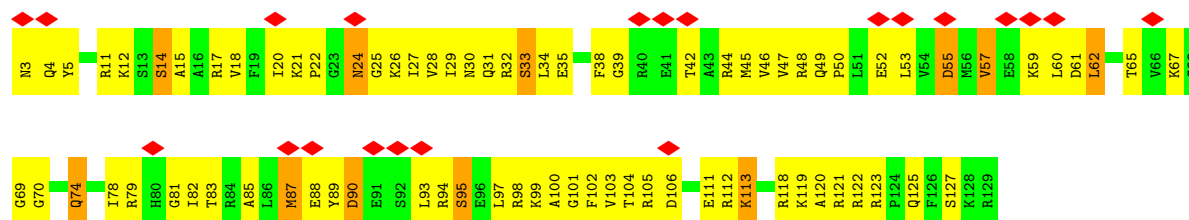
• Molecule 37: 30S ribosomal protein S7



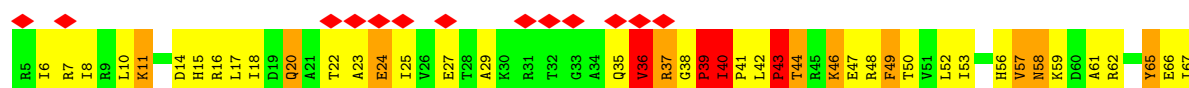
• Molecule 38: 30S ribosomal protein S8

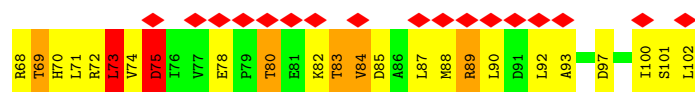


• Molecule 39: 30S ribosomal protein S9



• Molecule 40: 30S ribosomal protein S10

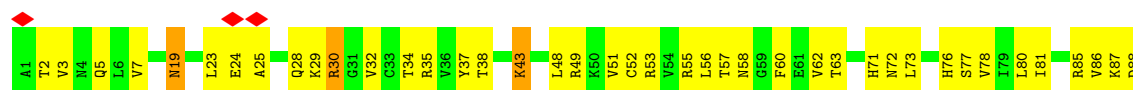




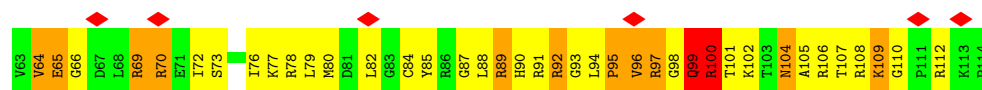
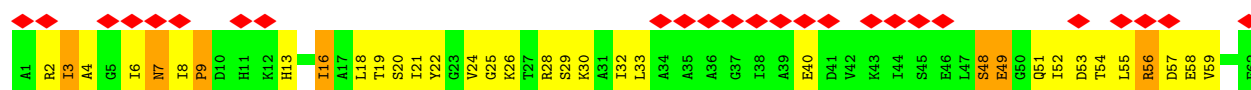
- Molecule 41: 30S ribosomal protein S11



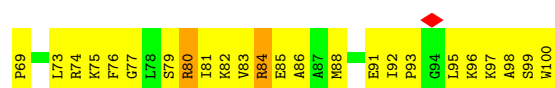
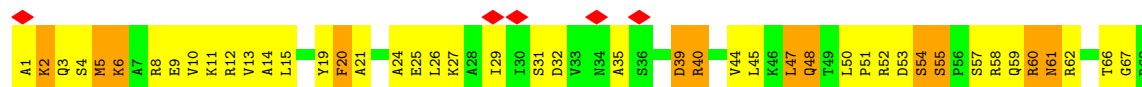
- Molecule 42: 30S ribosomal protein S12



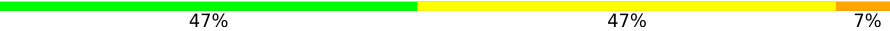
- Molecule 43: 30S ribosomal protein S13

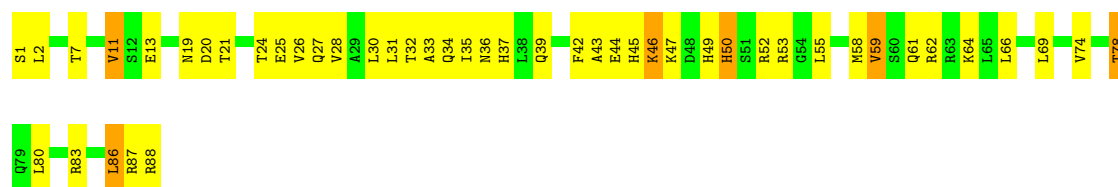


- Molecule 44: 30S ribosomal protein S14



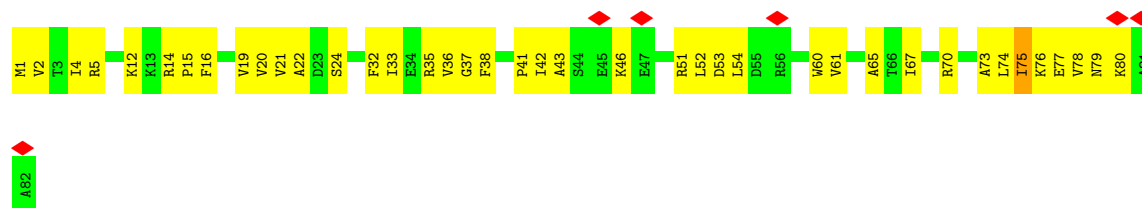
- Molecule 45: 30S ribosomal protein S15

Chain T: 



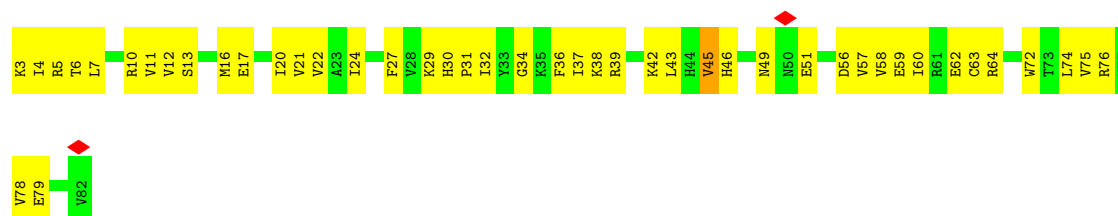
- Molecule 46: 30S ribosomal protein S16

Chain U: 



- Molecule 47: 30S ribosomal protein S17

Chain V: 



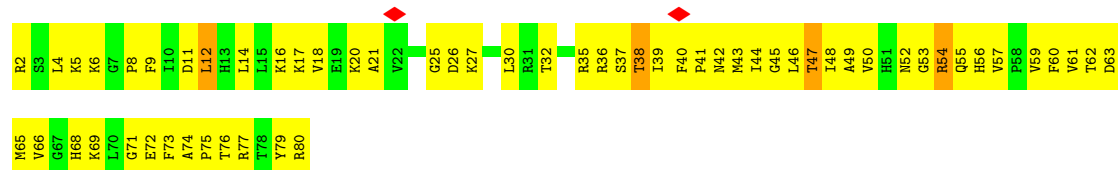
- Molecule 48: 30S ribosomal protein S18

Chain W: 



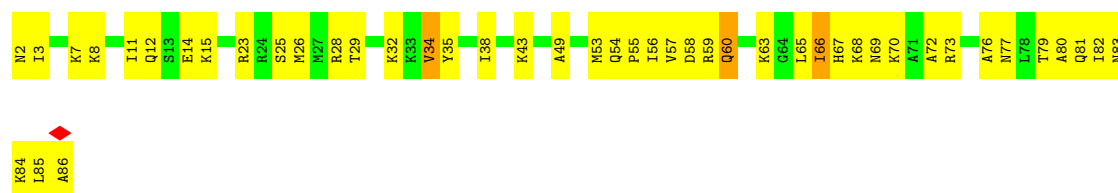
- Molecule 49: 30S ribosomal protein S19

Chain X: 



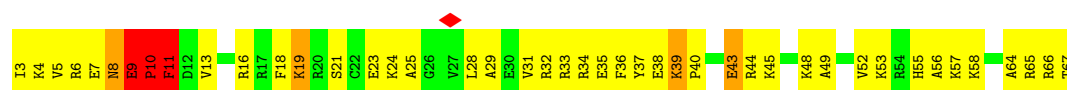
- Molecule 50: 30S ribosomal protein S20

Chain Y: 

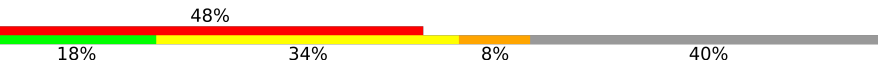


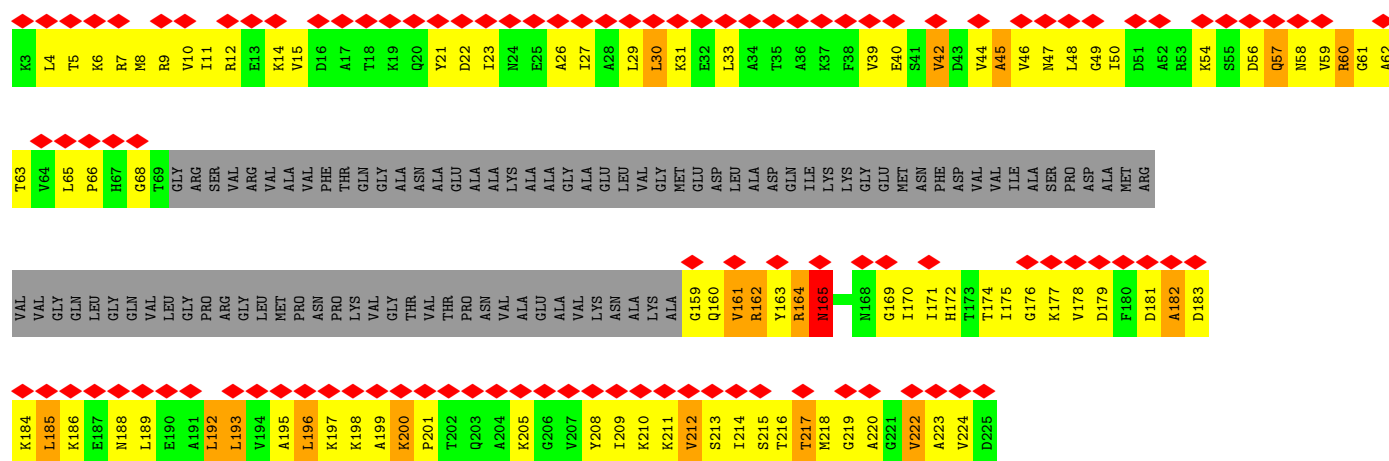
- Molecule 51: 30S ribosomal protein S21

Chain Z: 



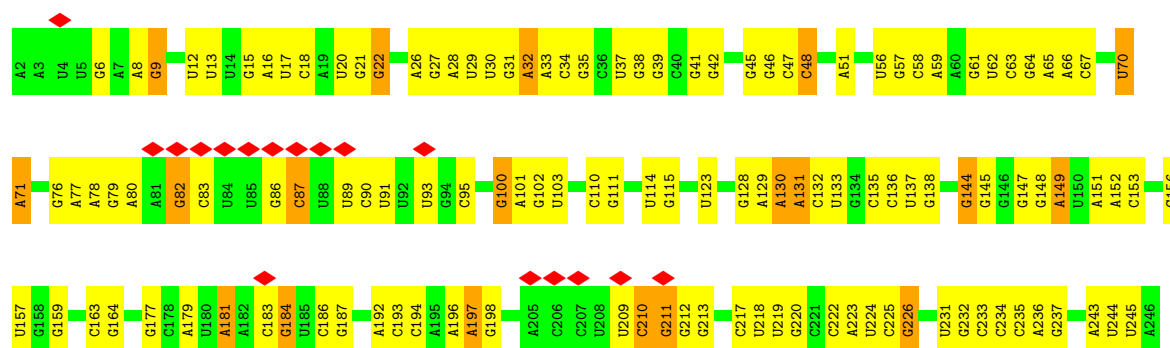
- Molecule 52: 50S ribosomal protein L1

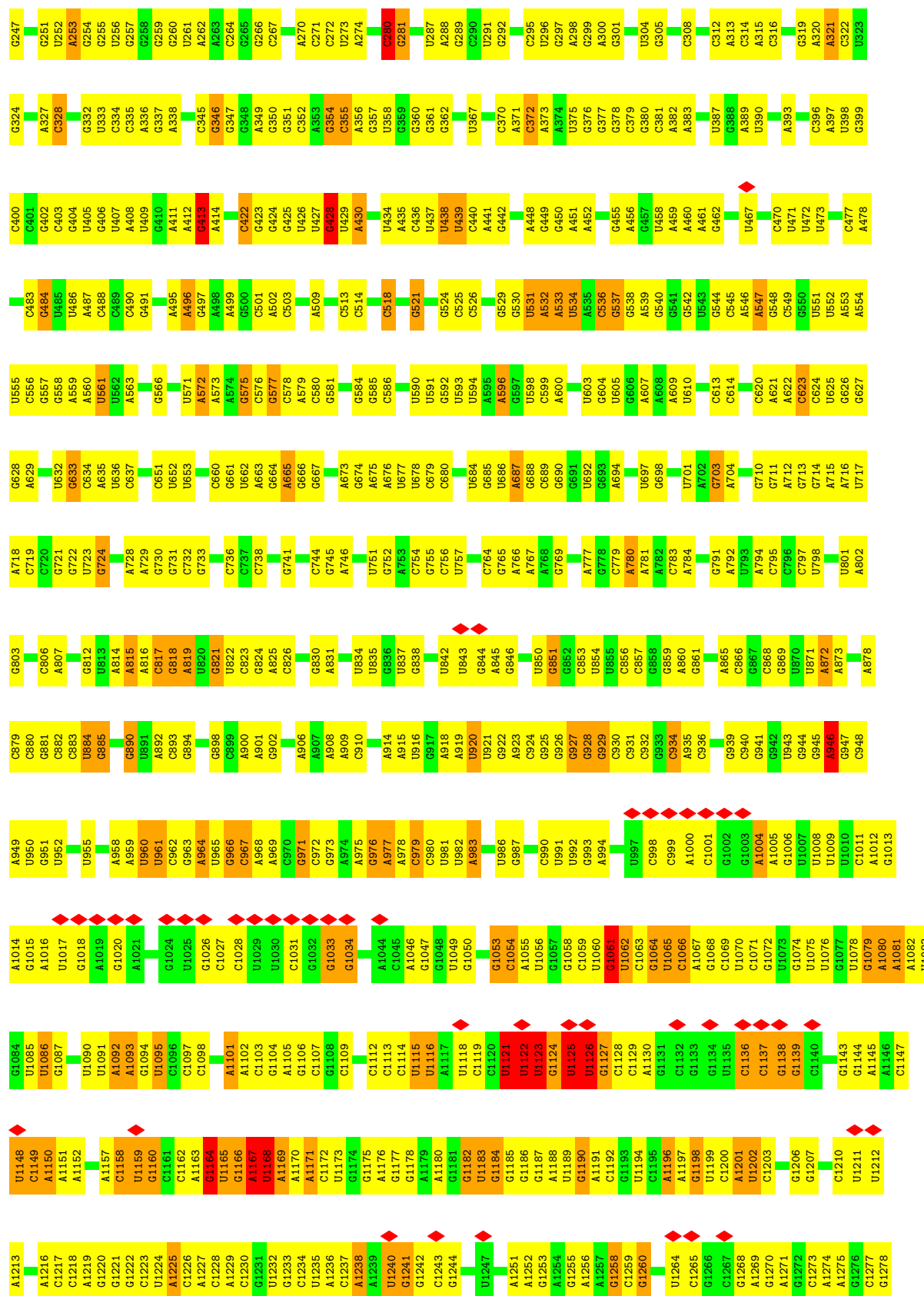
Chain a: 

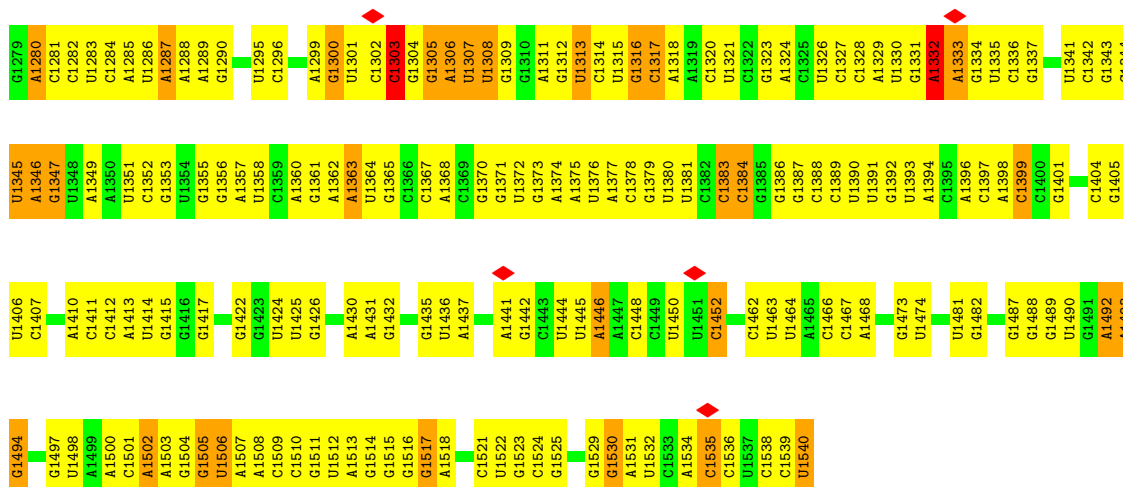


- Molecule 53: 16S ribosomal RNA

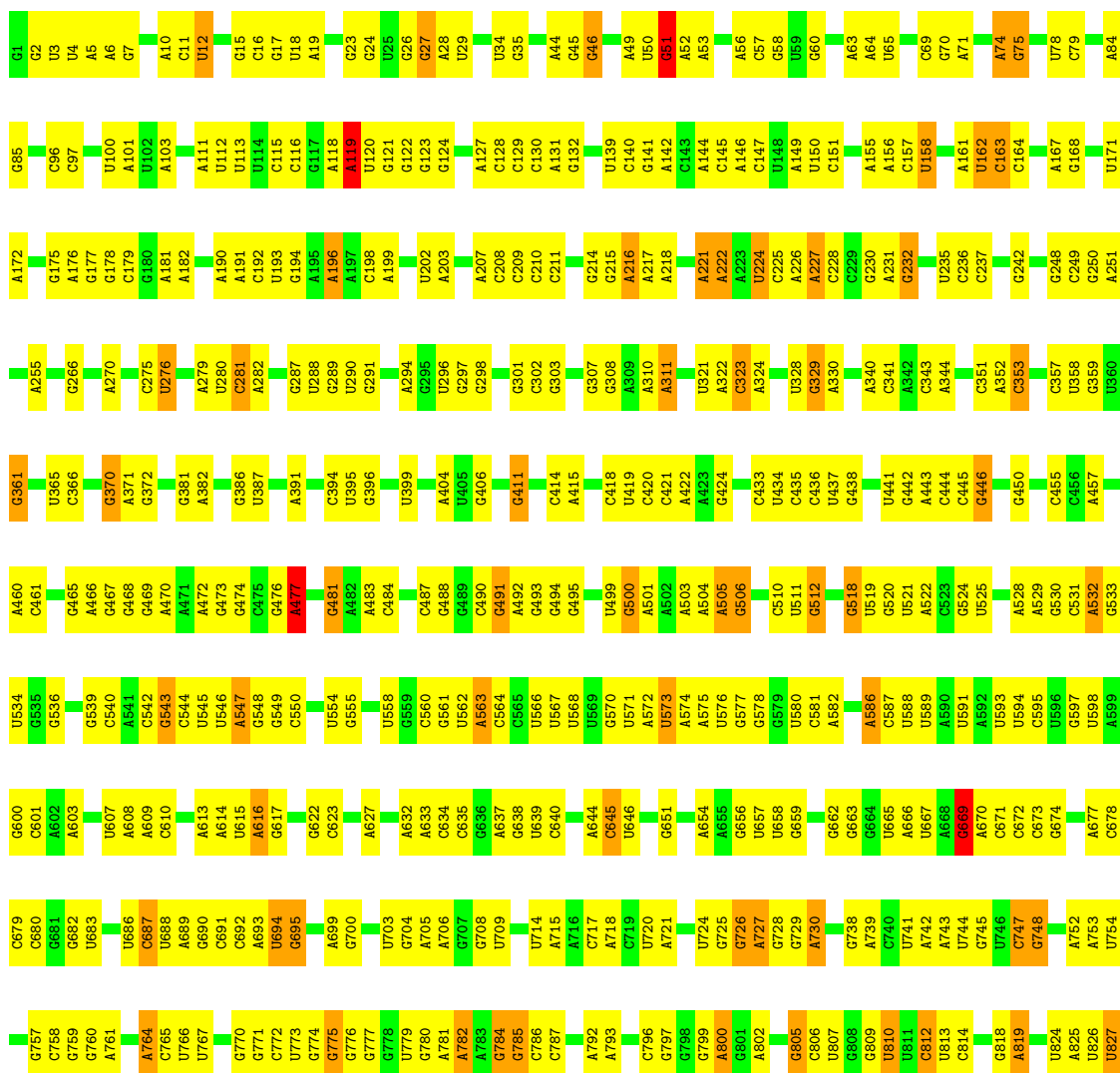
Chain 3: 

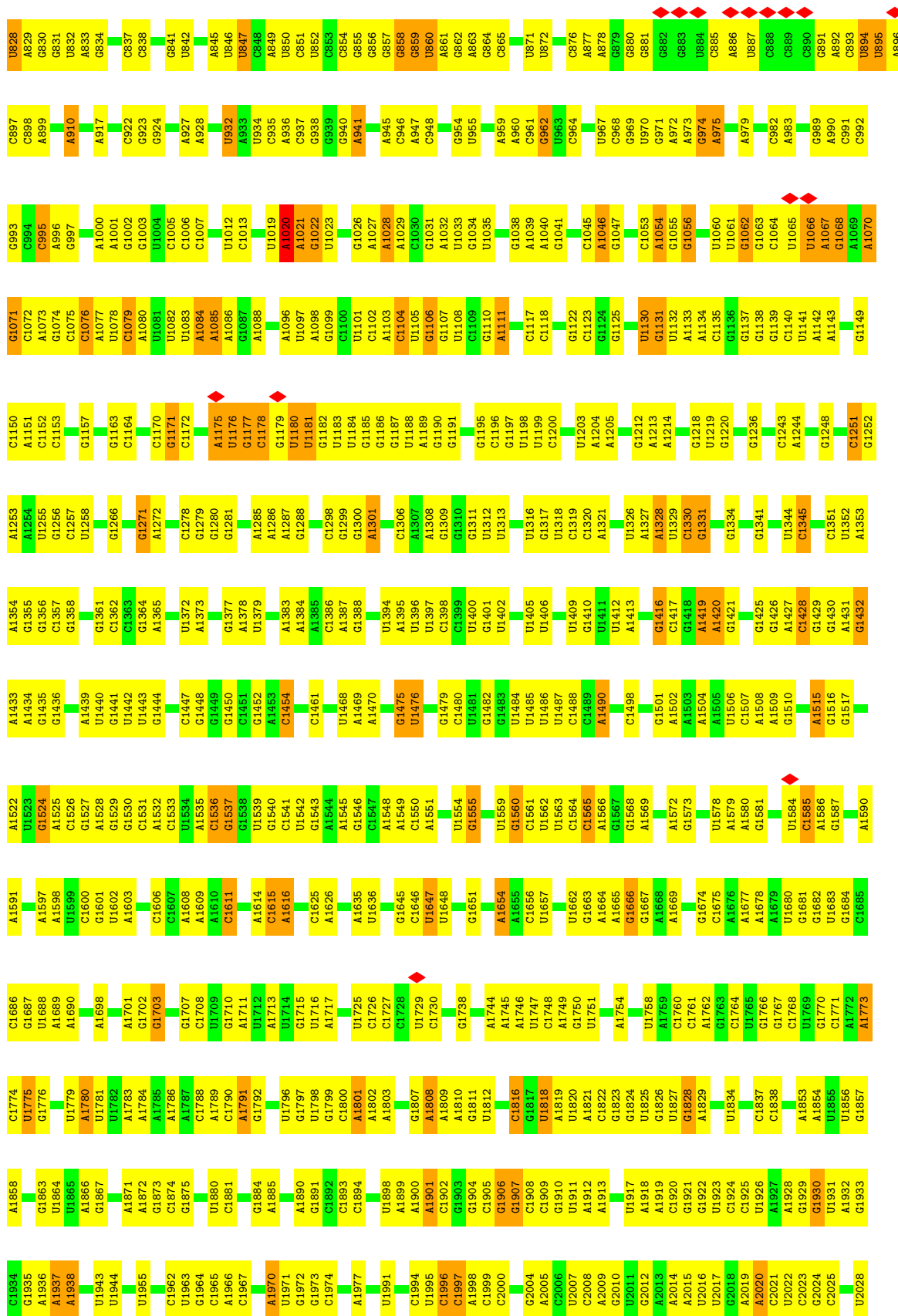


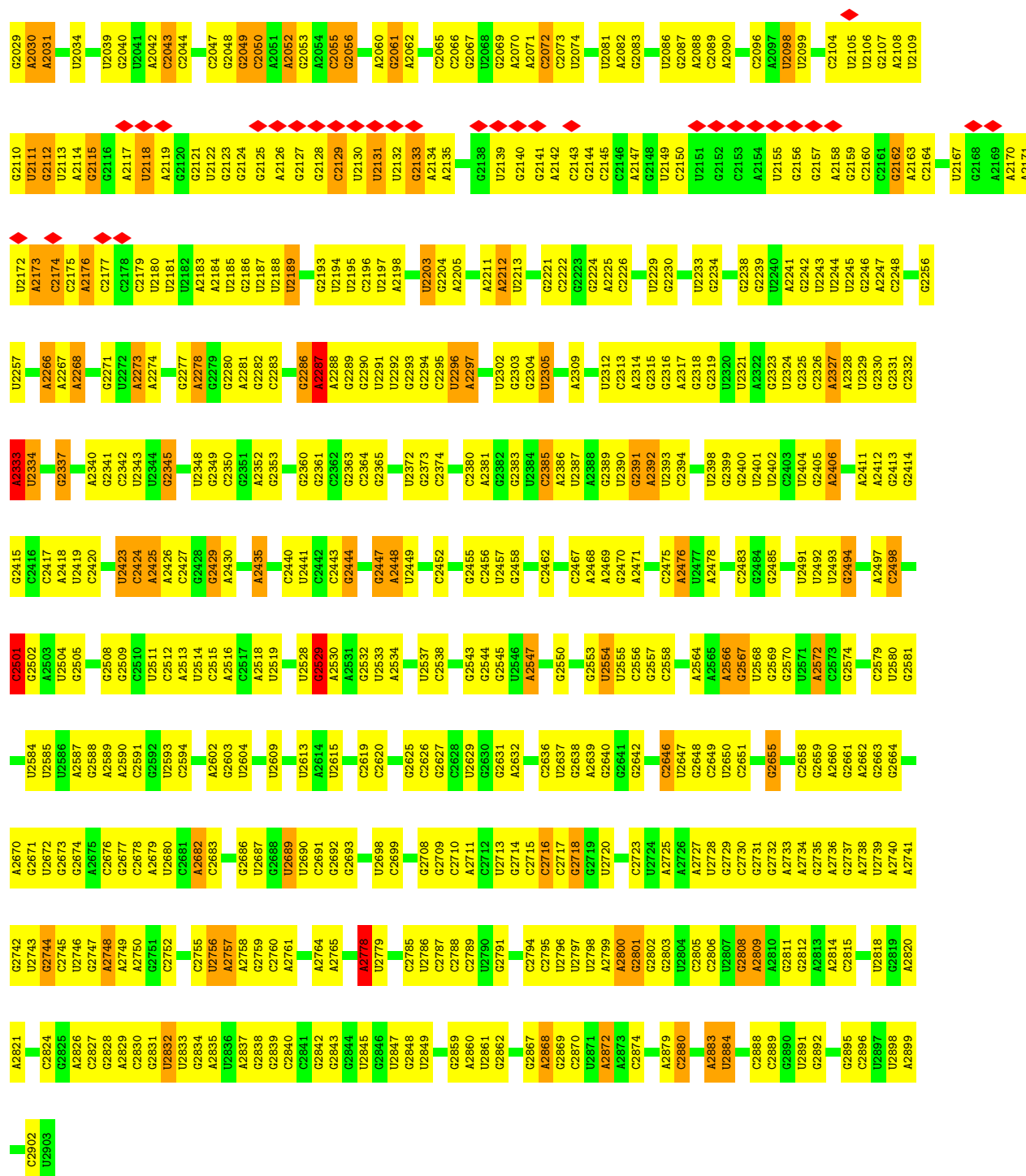




• Molecule 54: 23S ribosomal RNA



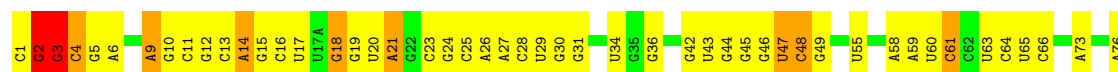
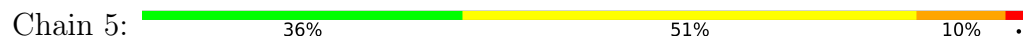




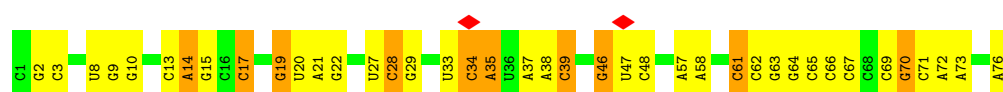




• Molecule 56: tRNA<sup>Pro</sup>



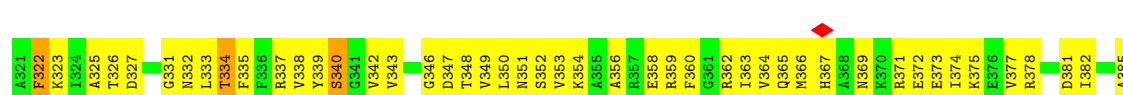
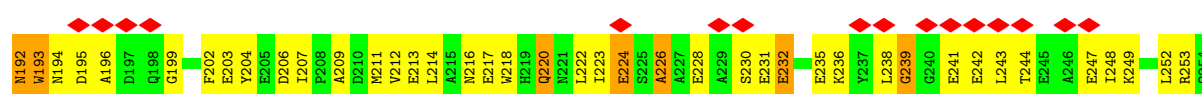
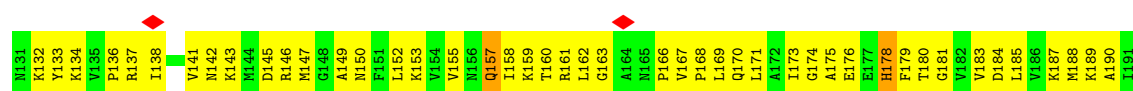
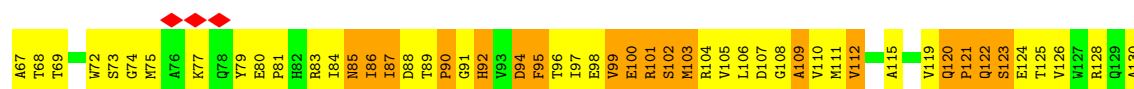
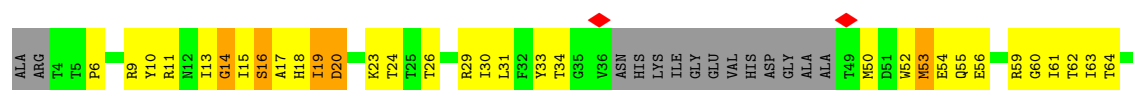
• Molecule 57: tRNA<sup>fMet</sup>

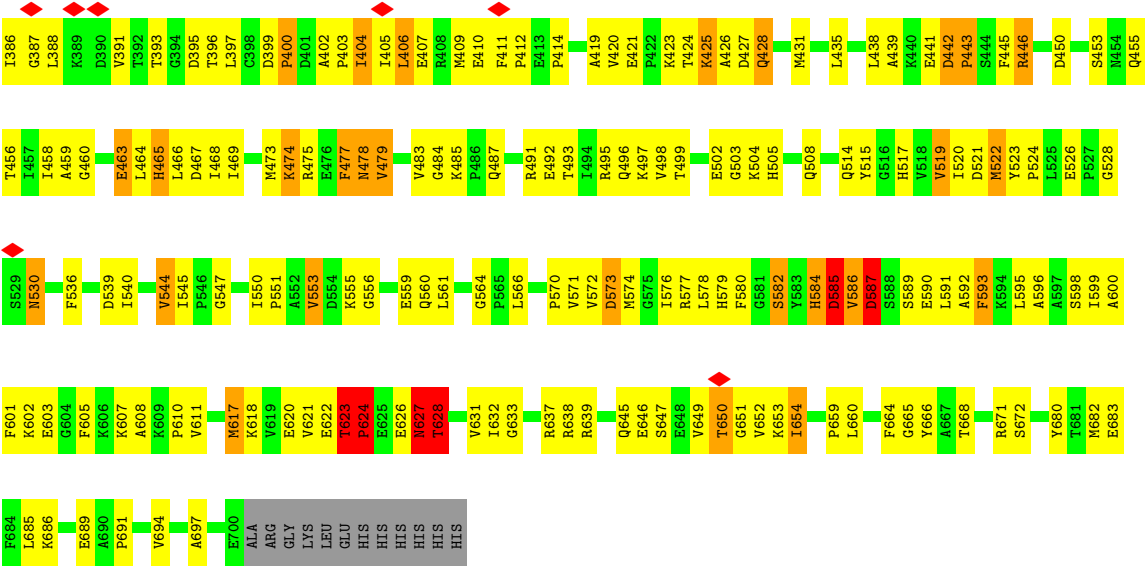


• Molecule 58: mRNA



• Molecule 59: Elongation factor G





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 9059                                    | 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 ( $e^-/\text{\AA}^2$ ) | 47.5                                    | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | 130000                                  | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 23.041                                  | Depositor |
| Minimum map value                    | -7.245                                  | Depositor |
| Average map value                    | 0.019                                   | Depositor |
| Map value standard deviation         | 1.364                                   | Depositor |
| Recommended contour level            | 3.7                                     | Depositor |
| Map size (Å)                         | 419.99997, 419.99997, 419.99997         | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.05, 1.05, 1.05                        | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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   | b     | 0.86         | 10/2122 (0.5%) | 1.10        | 12/2852 (0.4%) |
| 2   | c     | 0.82         | 3/1586 (0.2%)  | 1.04        | 7/2134 (0.3%)  |
| 3   | d     | 1.02         | 12/1571 (0.8%) | 1.08        | 13/2113 (0.6%) |
| 4   | e     | 0.90         | 9/1435 (0.6%)  | 1.10        | 14/1926 (0.7%) |
| 5   | f     | 0.85         | 8/1343 (0.6%)  | 1.03        | 8/1816 (0.4%)  |
| 6   | g     | 1.89         | 19/946 (2.0%)  | 1.53        | 26/1275 (2.0%) |
| 7   | h     | 1.53         | 13/638 (2.0%)  | 1.56        | 16/860 (1.9%)  |
| 8   | i     | 2.57         | 22/564 (3.9%)  | 1.89        | 28/768 (3.6%)  |
| 9   | j     | 0.75         | 4/1152 (0.3%)  | 0.92        | 6/1551 (0.4%)  |
| 10  | k     | 0.94         | 7/948 (0.7%)   | 1.24        | 12/1268 (0.9%) |
| 11  | l     | 0.77         | 4/1054 (0.4%)  | 1.08        | 6/1403 (0.4%)  |
| 12  | m     | 0.90         | 8/1093 (0.7%)  | 1.15        | 10/1460 (0.7%) |
| 13  | n     | 0.74         | 1/974 (0.1%)   | 1.05        | 6/1301 (0.5%)  |
| 14  | o     | 1.10         | 8/902 (0.9%)   | 1.11        | 5/1209 (0.4%)  |
| 15  | p     | 0.71         | 4/929 (0.4%)   | 0.88        | 0/1242         |
| 16  | q     | 0.76         | 3/960 (0.3%)   | 1.08        | 8/1278 (0.6%)  |
| 17  | r     | 0.74         | 3/829 (0.4%)   | 1.12        | 9/1107 (0.8%)  |
| 18  | s     | 1.10         | 9/864 (1.0%)   | 1.26        | 11/1156 (1.0%) |
| 19  | t     | 0.84         | 4/745 (0.5%)   | 0.95        | 3/994 (0.3%)   |
| 20  | u     | 0.70         | 2/788 (0.3%)   | 0.90        | 3/1051 (0.3%)  |
| 21  | v     | 0.79         | 3/766 (0.4%)   | 1.13        | 8/1025 (0.8%)  |
| 22  | w     | 0.74         | 1/582 (0.2%)   | 1.01        | 4/769 (0.5%)   |
| 23  | x     | 0.93         | 4/635 (0.6%)   | 1.22        | 5/848 (0.6%)   |
| 24  | y     | 0.99         | 4/510 (0.8%)   | 1.08        | 5/677 (0.7%)   |
| 25  | z     | 0.73         | 1/453 (0.2%)   | 0.90        | 0/605          |
| 26  | A     | 1.15         | 8/532 (1.5%)   | 1.25        | 10/709 (1.4%)  |
| 27  | B     | 0.57         | 0/450          | 0.83        | 0/599          |
| 28  | C     | 0.81         | 2/417 (0.5%)   | 1.00        | 3/554 (0.5%)   |
| 29  | D     | 0.65         | 0/380          | 0.93        | 1/498 (0.2%)   |
| 30  | E     | 0.76         | 2/513 (0.4%)   | 0.93        | 0/676          |
| 31  | F     | 0.85         | 1/303 (0.3%)   | 1.04        | 2/397 (0.5%)   |
| 32  | G     | 1.03         | 12/1736 (0.7%) | 1.18        | 14/2338 (0.6%) |

| Mol | Chain | Bond lengths |                   | Bond angles |                   |
|-----|-------|--------------|-------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5           | RMSZ        | # Z  >5           |
| 33  | H     | 1.23         | 18/1652 (1.1%)    | 1.20        | 13/2225 (0.6%)    |
| 34  | I     | 0.99         | 14/1665 (0.8%)    | 1.20        | 14/2227 (0.6%)    |
| 35  | J     | 1.03         | 8/1170 (0.7%)     | 1.19        | 12/1573 (0.8%)    |
| 36  | K     | 1.22         | 11/836 (1.3%)     | 1.27        | 9/1128 (0.8%)     |
| 37  | L     | 1.25         | 13/1196 (1.1%)    | 1.25        | 17/1602 (1.1%)    |
| 38  | M     | 0.94         | 5/989 (0.5%)      | 1.08        | 9/1326 (0.7%)     |
| 39  | N     | 1.00         | 8/1034 (0.8%)     | 1.17        | 10/1375 (0.7%)    |
| 40  | O     | 1.68         | 14/797 (1.8%)     | 1.41        | 13/1077 (1.2%)    |
| 41  | P     | 1.09         | 10/886 (1.1%)     | 1.28        | 12/1195 (1.0%)    |
| 42  | Q     | 0.78         | 2/969 (0.2%)      | 1.05        | 5/1300 (0.4%)     |
| 43  | R     | 1.37         | 12/893 (1.3%)     | 1.47        | 15/1193 (1.3%)    |
| 44  | S     | 1.21         | 10/817 (1.2%)     | 1.18        | 4/1088 (0.4%)     |
| 45  | T     | 0.97         | 5/722 (0.7%)      | 1.19        | 4/964 (0.4%)      |
| 46  | U     | 0.69         | 1/659 (0.2%)      | 0.91        | 1/884 (0.1%)      |
| 47  | V     | 0.57         | 0/658             | 0.94        | 2/881 (0.2%)      |
| 48  | W     | 1.26         | 6/545 (1.1%)      | 1.32        | 7/731 (1.0%)      |
| 49  | X     | 1.05         | 5/653 (0.8%)      | 1.15        | 2/877 (0.2%)      |
| 50  | Y     | 1.05         | 7/671 (1.0%)      | 1.12        | 6/888 (0.7%)      |
| 51  | Z     | 1.02         | 6/551 (1.1%)      | 1.37        | 11/728 (1.5%)     |
| 52  | a     | 2.21         | 33/1034 (3.2%)    | 1.68        | 37/1387 (2.7%)    |
| 53  | 3     | 0.55         | 0/36963           | 0.61        | 22/57662 (0.0%)   |
| 54  | 1     | 0.50         | 0/69796           | 0.57        | 18/108888 (0.0%)  |
| 55  | 2     | 0.48         | 0/2872            | 0.56        | 2/4479 (0.0%)     |
| 56  | 5     | 0.47         | 0/1840            | 0.61        | 1/2868 (0.0%)     |
| 57  | 6     | 0.49         | 0/1832            | 0.59        | 0/2855            |
| 58  | 4     | 0.72         | 1/388 (0.3%)      | 0.65        | 0/603             |
| 59  | 8     | 1.05         | 48/5411 (0.9%)    | 1.23        | 77/7323 (1.1%)    |
| All | All   | 0.74         | 428/166219 (0.3%) | 0.80        | 578/247786 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6   | g     | 0                   | 4                   |
| 34  | I     | 0                   | 1                   |
| 35  | J     | 0                   | 1                   |
| 53  | 3     | 0                   | 25                  |
| 54  | 1     | 0                   | 59                  |
| 55  | 2     | 0                   | 3                   |
| 56  | 5     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 59  | 8     | 0                   | 2                   |
| All | All   | 0                   | 96                  |

All (428) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 52  | a     | 59  | VAL  | C-O   | 33.06  | 1.59        | 1.24     |
| 6   | g     | 8   | LYS  | C-O   | -30.43 | 0.85        | 1.24     |
| 8   | i     | 56  | VAL  | C-O   | 26.89  | 1.52        | 1.23     |
| 40  | O     | 73  | LEU  | C-O   | 24.05  | 1.51        | 1.24     |
| 52  | a     | 163 | TYR  | C-O   | 21.83  | 1.51        | 1.23     |
| 8   | i     | 8   | VAL  | C-O   | 21.32  | 1.45        | 1.23     |
| 40  | O     | 75  | ASP  | C-O   | 20.63  | 1.47        | 1.23     |
| 6   | g     | 114 | GLU  | C-O   | 17.81  | 1.46        | 1.24     |
| 37  | L     | 104 | VAL  | C-O   | 17.76  | 1.44        | 1.24     |
| 8   | i     | 58  | ILE  | C-O   | 16.70  | 1.43        | 1.23     |
| 52  | a     | 61  | GLY  | C-O   | 15.60  | 1.39        | 1.23     |
| 52  | a     | 195 | ALA  | C-O   | 15.51  | 1.42        | 1.24     |
| 48  | W     | 12  | PHE  | C-O   | 15.22  | 1.43        | 1.24     |
| 8   | i     | 10  | LEU  | C-O   | 14.89  | 1.37        | 1.24     |
| 8   | i     | 54  | ILE  | C-O   | 14.57  | 1.42        | 1.24     |
| 36  | K     | 13  | ASP  | C-O   | 14.42  | 1.40        | 1.24     |
| 8   | i     | 57  | VAL  | C-O   | 14.06  | 1.39        | 1.24     |
| 3   | d     | 48  | THR  | C-O   | 13.76  | 1.38        | 1.23     |
| 6   | g     | 132 | PHE  | C-O   | 13.67  | 1.39        | 1.23     |
| 32  | G     | 83  | ALA  | C-O   | 13.52  | 1.40        | 1.24     |
| 35  | J     | 96  | GLN  | C-O   | 13.35  | 1.35        | 1.24     |
| 52  | a     | 181 | ASP  | C-O   | 13.01  | 1.41        | 1.23     |
| 33  | H     | 169 | GLU  | C-O   | 12.96  | 1.39        | 1.23     |
| 52  | a     | 161 | VAL  | C-O   | 12.94  | 1.37        | 1.23     |
| 2   | c     | 157 | LYS  | C-O   | 12.70  | 1.39        | 1.23     |
| 8   | i     | 9   | LYS  | C-N   | 12.50  | 1.45        | 1.33     |
| 49  | X     | 66  | VAL  | C-O   | 12.36  | 1.38        | 1.24     |
| 33  | H     | 154 | GLY  | C-O   | 12.31  | 1.40        | 1.23     |
| 14  | o     | 77  | ALA  | C-O   | 12.19  | 1.39        | 1.24     |
| 43  | R     | 16  | ILE  | C-O   | 12.12  | 1.37        | 1.24     |
| 14  | o     | 76  | LYS  | C-O   | 11.89  | 1.37        | 1.24     |
| 33  | H     | 199 | VAL  | C-O   | 11.79  | 1.36        | 1.23     |
| 40  | O     | 39  | PRO  | C-N   | 11.66  | 1.46        | 1.33     |
| 52  | a     | 213 | SER  | C-O   | 11.58  | 1.37        | 1.23     |
| 8   | i     | 57  | VAL  | C-N   | 11.43  | 1.46        | 1.33     |
| 7   | h     | 59  | LEU  | C-O   | 11.21  | 1.36        | 1.23     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | d     | 14  | VAL  | C-O   | 11.17 | 1.35        | 1.23     |
| 6   | g     | 49  | ALA  | C-O   | 11.10 | 1.33        | 1.23     |
| 59  | 8     | 100 | GLU  | C-O   | 11.09 | 1.36        | 1.24     |
| 32  | G     | 206 | ILE  | C-O   | 11.09 | 1.37        | 1.24     |
| 8   | i     | 8   | VAL  | N-CA  | 11.00 | 1.58        | 1.46     |
| 6   | g     | 43  | ASN  | C-O   | 10.96 | 1.38        | 1.24     |
| 59  | 8     | 623 | THR  | C-O   | 10.89 | 1.38        | 1.24     |
| 21  | v     | 92  | VAL  | N-CA  | 10.84 | 1.59        | 1.46     |
| 34  | I     | 155 | LYS  | N-CA  | 10.65 | 1.59        | 1.46     |
| 43  | R     | 89  | ARG  | C-O   | 10.62 | 1.36        | 1.24     |
| 39  | N     | 24  | ASN  | C-O   | 10.62 | 1.35        | 1.23     |
| 34  | I     | 69  | ARG  | C-O   | 10.59 | 1.36        | 1.24     |
| 52  | a     | 45  | ALA  | C-O   | 10.55 | 1.35        | 1.24     |
| 59  | 8     | 665 | GLY  | C-O   | 10.55 | 1.37        | 1.24     |
| 40  | O     | 80  | THR  | C-O   | 10.54 | 1.37        | 1.24     |
| 26  | A     | 45  | THR  | C-O   | 10.52 | 1.38        | 1.23     |
| 52  | a     | 63  | THR  | C-O   | 10.51 | 1.36        | 1.23     |
| 38  | M     | 35  | ILE  | C-O   | 10.47 | 1.36        | 1.24     |
| 3   | d     | 191 | ASP  | C-O   | 10.30 | 1.36        | 1.24     |
| 52  | a     | 165 | ASN  | N-CA  | 10.22 | 1.59        | 1.46     |
| 4   | e     | 7   | TYR  | C-O   | 10.14 | 1.35        | 1.24     |
| 59  | 8     | 650 | THR  | C-O   | 10.11 | 1.38        | 1.24     |
| 6   | g     | 101 | ASP  | C-O   | 10.08 | 1.35        | 1.24     |
| 6   | g     | 42  | LYS  | C-O   | 10.04 | 1.37        | 1.23     |
| 6   | g     | 126 | GLY  | C-O   | 9.97  | 1.37        | 1.23     |
| 22  | w     | 27  | VAL  | C-O   | 9.93  | 1.35        | 1.23     |
| 32  | G     | 139 | GLU  | C-O   | 9.92  | 1.35        | 1.24     |
| 31  | F     | 4   | ARG  | C-O   | 9.89  | 1.35        | 1.23     |
| 8   | i     | 27  | LEU  | C-O   | 9.84  | 1.36        | 1.24     |
| 24  | y     | 40  | SER  | C-O   | 9.74  | 1.36        | 1.24     |
| 41  | P     | 31  | VAL  | N-CA  | 9.69  | 1.57        | 1.46     |
| 33  | H     | 20  | THR  | C-O   | 9.66  | 1.35        | 1.24     |
| 52  | a     | 42  | VAL  | C-O   | 9.65  | 1.36        | 1.23     |
| 52  | a     | 164 | ARG  | C-N   | 9.57  | 1.47        | 1.33     |
| 5   | f     | 104 | LEU  | C-O   | 9.53  | 1.36        | 1.23     |
| 43  | R     | 56  | ARG  | C-O   | 9.47  | 1.35        | 1.24     |
| 59  | 8     | 589 | SER  | C-O   | 9.45  | 1.37        | 1.23     |
| 40  | O     | 37  | ARG  | N-CA  | 9.43  | 1.58        | 1.46     |
| 48  | W     | 55  | ALA  | C-O   | 9.42  | 1.34        | 1.24     |
| 8   | i     | 40  | ALA  | C-O   | 9.40  | 1.35        | 1.24     |
| 15  | p     | 6   | GLN  | C-O   | 9.40  | 1.35        | 1.24     |
| 18  | s     | 41  | LYS  | C-O   | 9.39  | 1.34        | 1.23     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 7   | h     | 25  | ALA  | C-O   | 9.36 | 1.35        | 1.23     |
| 59  | 8     | 101 | ARG  | C-O   | 9.32 | 1.34        | 1.24     |
| 48  | W     | 40  | PRO  | C-O   | 9.30 | 1.34        | 1.23     |
| 1   | b     | 210 | ALA  | C-O   | 9.25 | 1.35        | 1.24     |
| 14  | o     | 58  | ILE  | C-O   | 9.20 | 1.35        | 1.23     |
| 7   | h     | 57  | ASN  | C-O   | 9.19 | 1.34        | 1.23     |
| 43  | R     | 29  | SER  | C-O   | 9.16 | 1.35        | 1.24     |
| 37  | L     | 103 | ILE  | C-O   | 9.09 | 1.34        | 1.24     |
| 37  | L     | 108 | ARG  | N-CA  | 9.07 | 1.57        | 1.46     |
| 7   | h     | 7   | ASP  | C-O   | 9.03 | 1.34        | 1.24     |
| 59  | 8     | 95  | PHE  | C-O   | 9.02 | 1.36        | 1.23     |
| 52  | a     | 184 | LYS  | C-O   | 8.99 | 1.34        | 1.24     |
| 59  | 8     | 659 | PRO  | C-O   | 8.93 | 1.34        | 1.23     |
| 33  | H     | 128 | MET  | C-O   | 8.91 | 1.34        | 1.23     |
| 12  | m     | 116 | ALA  | C-O   | 8.84 | 1.34        | 1.24     |
| 59  | 8     | 14  | GLY  | C-O   | 8.84 | 1.35        | 1.23     |
| 18  | s     | 16  | LYS  | C-O   | 8.81 | 1.34        | 1.24     |
| 59  | 8     | 230 | SER  | N-CA  | 8.79 | 1.57        | 1.46     |
| 19  | t     | 4   | GLU  | C-O   | 8.76 | 1.35        | 1.24     |
| 26  | A     | 60  | PHE  | C-O   | 8.76 | 1.34        | 1.24     |
| 41  | P     | 18  | GLY  | C-O   | 8.68 | 1.30        | 1.24     |
| 59  | 8     | 312 | SER  | C-O   | 8.67 | 1.34        | 1.23     |
| 59  | 8     | 232 | GLU  | C-O   | 8.65 | 1.34        | 1.24     |
| 39  | N     | 15  | ALA  | N-CA  | 8.64 | 1.56        | 1.46     |
| 39  | N     | 33  | SER  | N-CA  | 8.63 | 1.57        | 1.45     |
| 59  | 8     | 628 | THR  | N-CA  | 8.59 | 1.57        | 1.46     |
| 52  | a     | 59  | VAL  | CA-C  | 8.55 | 1.63        | 1.52     |
| 52  | a     | 212 | VAL  | C-O   | 8.55 | 1.34        | 1.24     |
| 28  | C     | 25  | ASN  | C-O   | 8.52 | 1.33        | 1.23     |
| 23  | x     | 65  | THR  | C-O   | 8.46 | 1.33        | 1.24     |
| 52  | a     | 162 | ARG  | C-N   | 8.44 | 1.44        | 1.33     |
| 12  | m     | 119 | LEU  | C-O   | 8.44 | 1.34        | 1.24     |
| 7   | h     | 33  | VAL  | C-O   | 8.31 | 1.32        | 1.23     |
| 52  | a     | 164 | ARG  | C-O   | 8.30 | 1.33        | 1.23     |
| 6   | g     | 132 | PHE  | C-N   | 8.29 | 1.45        | 1.33     |
| 39  | N     | 67  | LYS  | C-O   | 8.28 | 1.33        | 1.24     |
| 26  | A     | 46  | GLY  | C-O   | 8.27 | 1.34        | 1.23     |
| 25  | z     | 42  | ALA  | C-O   | 8.26 | 1.33        | 1.24     |
| 59  | 8     | 150 | ASN  | C-O   | 8.21 | 1.33        | 1.24     |
| 43  | R     | 66  | GLY  | C-O   | 8.20 | 1.33        | 1.23     |
| 48  | W     | 12  | PHE  | CA-C  | 8.20 | 1.60        | 1.53     |
| 52  | a     | 196 | LEU  | C-O   | 8.16 | 1.34        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 33  | H     | 148 | ILE  | C-O   | 8.15  | 1.33        | 1.23     |
| 33  | H     | 184 | ASN  | C-O   | 8.14  | 1.33        | 1.23     |
| 36  | K     | 59  | TYR  | C-O   | 8.14  | 1.33        | 1.23     |
| 6   | g     | 100 | ALA  | C-O   | 8.13  | 1.33        | 1.24     |
| 11  | l     | 18  | ARG  | N-CA  | 8.10  | 1.55        | 1.46     |
| 44  | S     | 80  | ARG  | C-O   | 8.10  | 1.34        | 1.24     |
| 13  | n     | 17  | ARG  | C-O   | 8.07  | 1.33        | 1.24     |
| 33  | H     | 148 | ILE  | N-CA  | 8.05  | 1.54        | 1.46     |
| 52  | a     | 199 | ALA  | N-CA  | 8.03  | 1.55        | 1.46     |
| 3   | d     | 194 | LYS  | C-O   | 8.01  | 1.33        | 1.24     |
| 24  | y     | 19  | LEU  | C-O   | 8.01  | 1.34        | 1.24     |
| 45  | T     | 59  | VAL  | C-O   | 8.01  | 1.33        | 1.24     |
| 36  | K     | 67  | PRO  | C-O   | 7.94  | 1.33        | 1.23     |
| 33  | H     | 152 | VAL  | C-O   | 7.93  | 1.32        | 1.24     |
| 44  | S     | 40  | ARG  | C-O   | 7.93  | 1.34        | 1.24     |
| 59  | 8     | 180 | THR  | C-O   | 7.92  | 1.35        | 1.24     |
| 40  | O     | 46  | LYS  | N-CA  | 7.91  | 1.55        | 1.45     |
| 8   | i     | 42  | ASN  | C-O   | 7.90  | 1.33        | 1.24     |
| 34  | I     | 134 | TYR  | C-O   | 7.88  | 1.33        | 1.24     |
| 52  | a     | 192 | LEU  | C-O   | 7.84  | 1.33        | 1.24     |
| 50  | Y     | 60  | GLN  | C-O   | 7.82  | 1.33        | 1.24     |
| 6   | g     | 13  | GLY  | C-O   | -7.69 | 1.13        | 1.23     |
| 9   | j     | 69  | ARG  | C-O   | 7.68  | 1.33        | 1.24     |
| 41  | P     | 21  | HIS  | N-CA  | 7.67  | 1.55        | 1.46     |
| 36  | K     | 14  | GLN  | C-O   | 7.66  | 1.33        | 1.24     |
| 59  | 8     | 553 | VAL  | N-CA  | -7.61 | 1.37        | 1.46     |
| 41  | P     | 80  | ASN  | C-O   | 7.59  | 1.33        | 1.23     |
| 32  | G     | 50  | ASN  | C-O   | 7.56  | 1.32        | 1.24     |
| 48  | W     | 16  | GLY  | N-CA  | 7.55  | 1.56        | 1.45     |
| 45  | T     | 25  | GLU  | C-O   | 7.54  | 1.32        | 1.24     |
| 39  | N     | 62  | LEU  | C-O   | 7.53  | 1.33        | 1.23     |
| 59  | 8     | 112 | VAL  | N-CA  | 7.52  | 1.55        | 1.46     |
| 33  | H     | 81  | GLU  | C-O   | 7.51  | 1.32        | 1.24     |
| 6   | g     | 13  | GLY  | C-N   | -7.51 | 1.23        | 1.33     |
| 38  | M     | 124 | ILE  | C-O   | 7.51  | 1.32        | 1.24     |
| 36  | K     | 17  | GLN  | N-CA  | 7.50  | 1.56        | 1.46     |
| 12  | m     | 105 | MET  | C-O   | 7.49  | 1.33        | 1.23     |
| 52  | a     | 193 | LEU  | C-O   | 7.46  | 1.32        | 1.24     |
| 18  | s     | 42  | LYS  | C-O   | 7.42  | 1.32        | 1.24     |
| 44  | S     | 45  | LEU  | C-O   | 7.42  | 1.32        | 1.24     |
| 52  | a     | 185 | LEU  | N-CA  | 7.31  | 1.55        | 1.46     |
| 18  | s     | 35  | ILE  | C-O   | 7.25  | 1.31        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7   | h     | 57  | ASN  | N-CA  | 7.22  | 1.56        | 1.46     |
| 37  | L     | 71  | THR  | C-O   | 7.21  | 1.31        | 1.24     |
| 32  | G     | 51  | GLU  | C-O   | 7.18  | 1.32        | 1.24     |
| 6   | g     | 45  | GLU  | N-CA  | 7.15  | 1.54        | 1.46     |
| 18  | s     | 40  | ASN  | N-CA  | 7.12  | 1.55        | 1.46     |
| 43  | R     | 69  | ARG  | C-O   | 7.12  | 1.32        | 1.24     |
| 34  | I     | 154 | VAL  | C-N   | 7.12  | 1.43        | 1.33     |
| 3   | d     | 121 | VAL  | N-CA  | 7.10  | 1.55        | 1.46     |
| 51  | Z     | 5   | VAL  | C-O   | 7.10  | 1.32        | 1.23     |
| 14  | o     | 70  | ALA  | C-O   | 7.04  | 1.32        | 1.24     |
| 9   | j     | 27  | ARG  | C-O   | 7.03  | 1.32        | 1.24     |
| 50  | Y     | 57  | VAL  | C-O   | 7.03  | 1.32        | 1.24     |
| 50  | Y     | 58  | ASP  | C-O   | 7.00  | 1.33        | 1.24     |
| 12  | m     | 53  | MET  | C-O   | 7.00  | 1.32        | 1.24     |
| 14  | o     | 75  | GLY  | C-O   | 6.98  | 1.32        | 1.23     |
| 23  | x     | 50  | VAL  | N-CA  | 6.95  | 1.55        | 1.46     |
| 59  | 8     | 102 | SER  | C-O   | 6.94  | 1.32        | 1.24     |
| 59  | 8     | 617 | MET  | C-O   | 6.93  | 1.31        | 1.24     |
| 14  | o     | 80  | GLU  | N-CA  | 6.90  | 1.54        | 1.46     |
| 44  | S     | 14  | ALA  | C-O   | 6.90  | 1.32        | 1.24     |
| 58  | 4     | 14  | A    | O3'-P | -6.90 | 1.50        | 1.61     |
| 8   | i     | 13  | ALA  | C-O   | 6.84  | 1.32        | 1.24     |
| 1   | b     | 47  | ARG  | C-O   | 6.82  | 1.32        | 1.23     |
| 59  | 8     | 228 | GLU  | C-O   | -6.82 | 1.15        | 1.24     |
| 59  | 8     | 593 | PHE  | C-O   | 6.82  | 1.32        | 1.24     |
| 3   | d     | 132 | LYS  | C-O   | 6.82  | 1.31        | 1.24     |
| 37  | L     | 106 | ALA  | C-O   | 6.79  | 1.32        | 1.24     |
| 8   | i     | 11  | GLN  | C-N   | -6.79 | 1.24        | 1.33     |
| 52  | a     | 182 | ALA  | C-O   | 6.78  | 1.31        | 1.24     |
| 4   | e     | 9   | ASP  | C-O   | 6.77  | 1.32        | 1.23     |
| 39  | N     | 74  | GLN  | C-O   | 6.76  | 1.32        | 1.24     |
| 7   | h     | 6   | GLN  | C-O   | 6.76  | 1.32        | 1.24     |
| 37  | L     | 65  | LEU  | C-O   | 6.75  | 1.33        | 1.24     |
| 20  | u     | 8   | ASP  | N-CA  | 6.74  | 1.54        | 1.46     |
| 50  | Y     | 14  | GLU  | C-O   | 6.72  | 1.31        | 1.24     |
| 10  | k     | 45  | GLU  | C-O   | 6.71  | 1.32        | 1.23     |
| 6   | g     | 139 | PHE  | N-CA  | 6.71  | 1.54        | 1.45     |
| 43  | R     | 49  | GLU  | C-O   | 6.70  | 1.32        | 1.24     |
| 6   | g     | 144 | VAL  | C-O   | 6.69  | 1.31        | 1.24     |
| 59  | 8     | 628 | THR  | CA-C  | 6.69  | 1.61        | 1.52     |
| 44  | S     | 39  | ASP  | C-O   | 6.68  | 1.31        | 1.24     |
| 32  | G     | 138 | ARG  | C-O   | 6.66  | 1.31        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 34  | I     | 88  | ASN  | C-O   | 6.65  | 1.31        | 1.24     |
| 34  | I     | 152 | SER  | C-O   | -6.64 | 1.15        | 1.24     |
| 35  | J     | 67  | ARG  | C-O   | 6.63  | 1.31        | 1.24     |
| 59  | 8     | 544 | VAL  | C-O   | 6.62  | 1.34        | 1.24     |
| 1   | b     | 263 | ASP  | N-CA  | 6.61  | 1.54        | 1.46     |
| 51  | Z     | 39  | LYS  | C-O   | -6.61 | 1.18        | 1.24     |
| 38  | M     | 34  | ALA  | C-O   | 6.58  | 1.31        | 1.24     |
| 5   | f     | 69  | ALA  | C-O   | 6.57  | 1.31        | 1.24     |
| 4   | e     | 91  | ARG  | N-CA  | 6.54  | 1.54        | 1.45     |
| 12  | m     | 42  | THR  | N-CA  | 6.54  | 1.54        | 1.45     |
| 36  | K     | 68  | GLN  | C-O   | 6.54  | 1.31        | 1.24     |
| 37  | L     | 148 | LYS  | N-CA  | 6.53  | 1.53        | 1.46     |
| 59  | 8     | 622 | GLU  | C-O   | 6.53  | 1.31        | 1.23     |
| 1   | b     | 41  | GLY  | C-O   | 6.51  | 1.33        | 1.24     |
| 41  | P     | 67  | GLU  | C-O   | 6.51  | 1.32        | 1.24     |
| 46  | U     | 75  | ILE  | C-O   | 6.50  | 1.31        | 1.24     |
| 33  | H     | 30  | ASP  | C-O   | 6.48  | 1.31        | 1.24     |
| 33  | H     | 71  | ARG  | C-O   | 6.48  | 1.32        | 1.24     |
| 43  | R     | 20  | SER  | N-CA  | 6.48  | 1.54        | 1.46     |
| 3   | d     | 29  | HIS  | C-O   | 6.47  | 1.31        | 1.24     |
| 2   | c     | 203 | VAL  | N-CA  | 6.46  | 1.54        | 1.46     |
| 18  | s     | 3   | THR  | C-O   | 6.44  | 1.33        | 1.23     |
| 35  | J     | 48  | GLY  | C-O   | 6.43  | 1.31        | 1.24     |
| 44  | S     | 6   | LYS  | C-O   | 6.40  | 1.31        | 1.24     |
| 50  | Y     | 35  | TYR  | C-O   | 6.40  | 1.31        | 1.24     |
| 39  | N     | 87  | MET  | C-O   | 6.40  | 1.31        | 1.23     |
| 37  | L     | 44  | SER  | C-O   | 6.39  | 1.32        | 1.24     |
| 40  | O     | 29  | ALA  | C-O   | 6.36  | 1.30        | 1.24     |
| 4   | e     | 144 | LYS  | C-N   | 6.35  | 1.41        | 1.33     |
| 17  | r     | 75  | VAL  | N-CA  | 6.34  | 1.54        | 1.46     |
| 14  | o     | 82  | ALA  | C-O   | 6.33  | 1.31        | 1.24     |
| 33  | H     | 50  | SER  | C-O   | 6.31  | 1.32        | 1.23     |
| 52  | a     | 175 | ILE  | N-CA  | 6.29  | 1.52        | 1.46     |
| 34  | I     | 60  | VAL  | C-O   | 6.29  | 1.31        | 1.24     |
| 49  | X     | 48  | ILE  | C-O   | 6.28  | 1.30        | 1.24     |
| 40  | O     | 11  | LYS  | C-O   | 6.26  | 1.31        | 1.23     |
| 26  | A     | 49  | ARG  | N-CA  | 6.26  | 1.54        | 1.46     |
| 10  | k     | 9   | ASN  | C-O   | 6.24  | 1.31        | 1.24     |
| 51  | Z     | 57  | LYS  | C-O   | 6.22  | 1.32        | 1.24     |
| 3   | d     | 179 | SER  | C-O   | 6.21  | 1.31        | 1.24     |
| 40  | O     | 84  | VAL  | N-CA  | 6.20  | 1.54        | 1.46     |
| 37  | L     | 36  | SER  | C-O   | 6.19  | 1.31        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 41  | P     | 66  | ALA  | C-O   | 6.17 | 1.31        | 1.24     |
| 59  | 8     | 463 | GLU  | C-O   | 6.17 | 1.31        | 1.24     |
| 44  | S     | 48  | GLN  | N-CA  | 6.16 | 1.53        | 1.46     |
| 35  | J     | 127 | TYR  | N-CA  | 6.14 | 1.53        | 1.45     |
| 35  | J     | 113 | VAL  | C-O   | 6.14 | 1.32        | 1.24     |
| 18  | s     | 106 | VAL  | C-O   | 6.12 | 1.30        | 1.24     |
| 34  | I     | 70  | GLN  | C-O   | 6.12 | 1.31        | 1.24     |
| 8   | i     | 9   | LYS  | C-O   | 6.12 | 1.31        | 1.24     |
| 14  | o     | 34  | HIS  | C-O   | 6.11 | 1.31        | 1.24     |
| 59  | 8     | 249 | LYS  | C-O   | 6.11 | 1.31        | 1.24     |
| 19  | t     | 86  | THR  | C-O   | 6.09 | 1.31        | 1.24     |
| 33  | H     | 159 | ALA  | N-CA  | 6.09 | 1.54        | 1.46     |
| 52  | a     | 57  | GLN  | N-CA  | 6.08 | 1.53        | 1.46     |
| 40  | O     | 40  | ILE  | N-CA  | 6.08 | 1.54        | 1.46     |
| 59  | 8     | 307 | ALA  | N-CA  | 6.08 | 1.54        | 1.45     |
| 4   | e     | 149 | ARG  | C-O   | 6.07 | 1.31        | 1.24     |
| 38  | M     | 84  | ILE  | C-O   | 6.07 | 1.30        | 1.24     |
| 24  | y     | 44  | LYS  | N-CA  | 6.06 | 1.53        | 1.46     |
| 37  | L     | 57  | GLU  | C-O   | 6.06 | 1.31        | 1.24     |
| 40  | O     | 65  | TYR  | C-O   | 6.06 | 1.30        | 1.24     |
| 7   | h     | 44  | ALA  | C-O   | 6.06 | 1.31        | 1.24     |
| 37  | L     | 120 | ALA  | C-O   | 6.05 | 1.31        | 1.24     |
| 51  | Z     | 11  | PHE  | N-CA  | 6.05 | 1.53        | 1.46     |
| 15  | p     | 3   | ILE  | C-O   | 6.05 | 1.31        | 1.24     |
| 2   | c     | 64  | GLU  | C-O   | 6.05 | 1.31        | 1.24     |
| 52  | a     | 212 | VAL  | C-N   | 6.04 | 1.42        | 1.33     |
| 20  | u     | 11  | ILE  | C-O   | 6.03 | 1.30        | 1.24     |
| 51  | Z     | 9   | GLU  | CA-C  | 6.03 | 1.60        | 1.52     |
| 48  | W     | 53  | GLN  | C-O   | 6.01 | 1.31        | 1.24     |
| 5   | f     | 114 | HIS  | N-CA  | 5.99 | 1.53        | 1.45     |
| 44  | S     | 84  | ARG  | C-O   | 5.99 | 1.31        | 1.24     |
| 32  | G     | 141 | GLU  | C-O   | 5.99 | 1.31        | 1.24     |
| 33  | H     | 146 | LYS  | C-O   | 5.99 | 1.31        | 1.24     |
| 52  | a     | 162 | ARG  | C-O   | 5.98 | 1.31        | 1.24     |
| 33  | H     | 155 | ARG  | C-O   | 5.96 | 1.33        | 1.23     |
| 9   | j     | 7   | LYS  | C-O   | 5.96 | 1.33        | 1.24     |
| 44  | S     | 11  | LYS  | C-O   | 5.93 | 1.31        | 1.24     |
| 17  | r     | 4   | VAL  | C-O   | 5.90 | 1.30        | 1.24     |
| 6   | g     | 30  | LEU  | C-O   | 5.88 | 1.30        | 1.24     |
| 51  | Z     | 19  | LYS  | C-O   | 5.88 | 1.30        | 1.24     |
| 43  | R     | 70  | ARG  | C-O   | 5.88 | 1.31        | 1.24     |
| 50  | Y     | 66  | ILE  | N-CA  | 5.87 | 1.53        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 8   | i     | 16  | MET  | N-CA  | 5.86  | 1.53        | 1.45     |
| 1   | b     | 203 | VAL  | N-CA  | 5.85  | 1.52        | 1.46     |
| 59  | 8     | 456 | THR  | C-O   | 5.85  | 1.31        | 1.24     |
| 33  | H     | 91  | ALA  | C-O   | 5.84  | 1.30        | 1.24     |
| 34  | I     | 61  | ARG  | C-O   | 5.83  | 1.31        | 1.24     |
| 50  | Y     | 34  | VAL  | C-O   | 5.83  | 1.31        | 1.24     |
| 26  | A     | 13  | THR  | C-N   | 5.82  | 1.41        | 1.33     |
| 34  | I     | 158 | LEU  | C-O   | 5.82  | 1.30        | 1.24     |
| 23  | x     | 48  | LEU  | N-CA  | 5.81  | 1.53        | 1.45     |
| 7   | h     | 37  | LYS  | N-CA  | 5.80  | 1.53        | 1.46     |
| 7   | h     | 64  | VAL  | N-CA  | 5.79  | 1.53        | 1.46     |
| 16  | q     | 7   | VAL  | C-O   | 5.79  | 1.30        | 1.24     |
| 17  | r     | 60  | LYS  | N-CA  | 5.79  | 1.52        | 1.45     |
| 36  | K     | 10  | VAL  | C-O   | 5.78  | 1.29        | 1.24     |
| 28  | C     | 11  | VAL  | N-CA  | 5.77  | 1.53        | 1.46     |
| 12  | m     | 35  | ALA  | C-O   | 5.76  | 1.31        | 1.23     |
| 34  | I     | 155 | LYS  | C-O   | 5.76  | 1.30        | 1.24     |
| 45  | T     | 78  | THR  | C-O   | 5.75  | 1.31        | 1.24     |
| 5   | f     | 11  | PRO  | C-O   | 5.75  | 1.30        | 1.23     |
| 59  | 8     | 428 | GLN  | N-CA  | 5.75  | 1.53        | 1.46     |
| 34  | I     | 186 | GLU  | N-CA  | 5.74  | 1.52        | 1.45     |
| 3   | d     | 187 | VAL  | C-O   | 5.74  | 1.30        | 1.23     |
| 8   | i     | 27  | LEU  | CA-C  | 5.73  | 1.60        | 1.52     |
| 52  | a     | 165 | ASN  | CA-C  | 5.73  | 1.60        | 1.52     |
| 35  | J     | 50  | GLY  | C-O   | 5.72  | 1.31        | 1.23     |
| 26  | A     | 47  | LYS  | C-O   | 5.71  | 1.31        | 1.24     |
| 42  | Q     | 97  | VAL  | C-O   | 5.71  | 1.29        | 1.24     |
| 23  | x     | 52  | ALA  | C-O   | 5.70  | 1.30        | 1.24     |
| 9   | j     | 81  | ILE  | N-CA  | 5.70  | 1.53        | 1.46     |
| 35  | J     | 123 | LEU  | C-O   | 5.68  | 1.30        | 1.23     |
| 59  | 8     | 110 | VAL  | N-CA  | 5.68  | 1.54        | 1.46     |
| 1   | b     | 16  | VAL  | C-O   | 5.68  | 1.30        | 1.24     |
| 30  | E     | 54  | LEU  | C-O   | 5.67  | 1.30        | 1.24     |
| 1   | b     | 92  | LEU  | C-O   | 5.67  | 1.30        | 1.24     |
| 24  | y     | 25  | GLN  | C-O   | 5.65  | 1.30        | 1.24     |
| 42  | Q     | 30  | ARG  | C-O   | 5.63  | 1.30        | 1.23     |
| 6   | g     | 46  | PHE  | N-CA  | 5.63  | 1.53        | 1.46     |
| 21  | v     | 73  | LYS  | C-O   | 5.62  | 1.31        | 1.23     |
| 41  | P     | 30  | ILE  | C-N   | -5.61 | 1.25        | 1.33     |
| 4   | e     | 53  | ALA  | C-O   | 5.61  | 1.30        | 1.24     |
| 32  | G     | 46  | VAL  | C-O   | 5.60  | 1.29        | 1.24     |
| 6   | g     | 40  | THR  | N-CA  | 5.60  | 1.54        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 18  | s     | 105 | VAL  | C-O   | 5.60  | 1.29        | 1.24     |
| 45  | T     | 50  | HIS  | C-O   | 5.58  | 1.30        | 1.24     |
| 59  | 8     | 654 | ILE  | N-CA  | 5.58  | 1.52        | 1.46     |
| 36  | K     | 29  | ILE  | C-O   | 5.57  | 1.30        | 1.24     |
| 43  | R     | 7   | ASN  | C-O   | 5.57  | 1.30        | 1.23     |
| 5   | f     | 34  | ARG  | C-O   | 5.57  | 1.30        | 1.23     |
| 59  | 8     | 624 | PRO  | C-N   | -5.56 | 1.25        | 1.33     |
| 6   | g     | 43  | ASN  | C-N   | 5.54  | 1.41        | 1.33     |
| 40  | O     | 24  | GLU  | C-O   | 5.53  | 1.30        | 1.24     |
| 59  | 8     | 479 | VAL  | N-CA  | 5.53  | 1.53        | 1.46     |
| 59  | 8     | 87  | ILE  | N-CA  | 5.52  | 1.53        | 1.46     |
| 36  | K     | 51  | ILE  | N-CA  | 5.50  | 1.53        | 1.46     |
| 8   | i     | 44  | LYS  | N-CA  | 5.50  | 1.54        | 1.45     |
| 39  | N     | 95  | SER  | C-O   | 5.50  | 1.30        | 1.24     |
| 10  | k     | 63  | VAL  | N-CA  | 5.49  | 1.51        | 1.46     |
| 4   | e     | 167 | ALA  | C-O   | 5.49  | 1.30        | 1.24     |
| 8   | i     | 58  | ILE  | C-N   | 5.47  | 1.40        | 1.33     |
| 16  | q     | 31  | TYR  | N-CA  | 5.47  | 1.52        | 1.46     |
| 3   | d     | 109 | LEU  | C-O   | 5.46  | 1.30        | 1.24     |
| 7   | h     | 17  | GLU  | C-O   | 5.46  | 1.31        | 1.24     |
| 38  | M     | 42  | GLU  | C-O   | 5.46  | 1.31        | 1.24     |
| 10  | k     | 17  | ARG  | C-O   | 5.45  | 1.31        | 1.23     |
| 7   | h     | 11  | ILE  | N-CA  | 5.45  | 1.52        | 1.46     |
| 32  | G     | 142 | LYS  | C-O   | 5.44  | 1.30        | 1.24     |
| 59  | 8     | 264 | VAL  | C-O   | 5.43  | 1.30        | 1.24     |
| 21  | v     | 69  | GLU  | N-CA  | 5.42  | 1.53        | 1.46     |
| 59  | 8     | 519 | VAL  | C-O   | 5.40  | 1.29        | 1.23     |
| 59  | 8     | 584 | HIS  | C-O   | 5.39  | 1.30        | 1.23     |
| 1   | b     | 260 | LYS  | C-O   | -5.38 | 1.17        | 1.24     |
| 41  | P     | 45  | THR  | C-O   | 5.38  | 1.30        | 1.23     |
| 33  | H     | 182 | ASP  | C-O   | 5.37  | 1.30        | 1.23     |
| 19  | t     | 63  | VAL  | C-O   | 5.37  | 1.29        | 1.24     |
| 10  | k     | 115 | ILE  | C-O   | 5.37  | 1.30        | 1.24     |
| 11  | l     | 141 | LYS  | C-O   | 5.37  | 1.30        | 1.23     |
| 59  | 8     | 157 | GLN  | C-O   | 5.35  | 1.30        | 1.24     |
| 26  | A     | 12  | ILE  | C-O   | 5.34  | 1.29        | 1.23     |
| 16  | q     | 79  | ILE  | C-O   | 5.33  | 1.31        | 1.24     |
| 5   | f     | 148 | ARG  | C-O   | 5.33  | 1.30        | 1.24     |
| 5   | f     | 85  | LYS  | C-O   | 5.32  | 1.30        | 1.24     |
| 15  | p     | 20  | ARG  | C-O   | 5.32  | 1.30        | 1.23     |
| 45  | T     | 11  | VAL  | C-O   | 5.32  | 1.30        | 1.24     |
| 10  | k     | 25  | LEU  | N-CA  | 5.31  | 1.52        | 1.45     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11  | l     | 135 | ILE  | C-O   | 5.30  | 1.30        | 1.24     |
| 59  | 8     | 99  | VAL  | N-CA  | 5.30  | 1.52        | 1.46     |
| 59  | 8     | 16  | SER  | C-O   | 5.29  | 1.29        | 1.24     |
| 26  | A     | 45  | THR  | CA-C  | 5.28  | 1.60        | 1.52     |
| 34  | I     | 129 | VAL  | N-CA  | 5.27  | 1.52        | 1.46     |
| 5   | f     | 70  | LEU  | C-O   | 5.26  | 1.30        | 1.24     |
| 19  | t     | 41  | ALA  | C-O   | 5.26  | 1.30        | 1.24     |
| 32  | G     | 181 | PRO  | C-O   | 5.26  | 1.29        | 1.23     |
| 49  | X     | 47  | THR  | N-CA  | 5.25  | 1.52        | 1.46     |
| 43  | R     | 3   | ILE  | C-O   | 5.24  | 1.30        | 1.23     |
| 40  | O     | 49  | PHE  | N-CA  | 5.24  | 1.52        | 1.46     |
| 8   | i     | 11  | GLN  | C-O   | -5.24 | 1.17        | 1.24     |
| 10  | k     | 113 | MET  | N-CA  | 5.24  | 1.52        | 1.46     |
| 32  | G     | 198 | VAL  | N-CA  | 5.22  | 1.52        | 1.46     |
| 36  | K     | 18  | VAL  | N-CA  | 5.21  | 1.52        | 1.46     |
| 59  | 8     | 96  | THR  | N-CA  | 5.20  | 1.52        | 1.46     |
| 59  | 8     | 193 | TRP  | N-CA  | 5.20  | 1.52        | 1.45     |
| 59  | 8     | 279 | LEU  | C-O   | 5.20  | 1.30        | 1.24     |
| 37  | L     | 5   | VAL  | N-CA  | 5.20  | 1.52        | 1.46     |
| 15  | p     | 26  | GLU  | C-O   | 5.19  | 1.29        | 1.24     |
| 49  | X     | 38  | THR  | C-N   | 5.18  | 1.41        | 1.33     |
| 44  | S     | 81  | ILE  | C-O   | 5.18  | 1.29        | 1.24     |
| 3   | d     | 36  | ALA  | C-O   | 5.17  | 1.30        | 1.24     |
| 41  | P     | 31  | VAL  | CA-C  | 5.17  | 1.58        | 1.52     |
| 3   | d     | 14  | VAL  | N-CA  | 5.16  | 1.51        | 1.46     |
| 12  | m     | 100 | LYS  | N-CA  | 5.16  | 1.52        | 1.46     |
| 59  | 8     | 367 | HIS  | N-CA  | 5.16  | 1.52        | 1.46     |
| 1   | b     | 116 | GLN  | C-O   | 5.15  | 1.28        | 1.24     |
| 1   | b     | 174 | ARG  | C-O   | 5.15  | 1.30        | 1.24     |
| 36  | K     | 43  | GLY  | N-CA  | 5.15  | 1.50        | 1.45     |
| 52  | a     | 176 | GLY  | C-O   | 5.15  | 1.30        | 1.24     |
| 52  | a     | 60  | ARG  | C-N   | 5.15  | 1.40        | 1.33     |
| 37  | L     | 134 | VAL  | C-O   | 5.14  | 1.30        | 1.24     |
| 49  | X     | 12  | LEU  | C-O   | 5.14  | 1.30        | 1.24     |
| 59  | 8     | 124 | GLU  | C-O   | 5.14  | 1.30        | 1.24     |
| 11  | l     | 94  | THR  | C-O   | -5.12 | 1.17        | 1.24     |
| 43  | R     | 48  | SER  | C-O   | 5.11  | 1.30        | 1.23     |
| 30  | E     | 53  | ASP  | C-O   | 5.10  | 1.30        | 1.24     |
| 59  | 8     | 110 | VAL  | C-O   | 5.09  | 1.29        | 1.24     |
| 52  | a     | 44  | VAL  | C-O   | 5.09  | 1.29        | 1.24     |
| 7   | h     | 75  | ALA  | C-O   | 5.08  | 1.30        | 1.24     |
| 4   | e     | 54  | ALA  | C-O   | 5.08  | 1.30        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 59  | 8     | 92  | HIS  | N-CA  | 5.08  | 1.53        | 1.46     |
| 8   | i     | 69  | VAL  | N-CA  | 5.08  | 1.52        | 1.46     |
| 35  | J     | 11  | GLN  | C-O   | 5.07  | 1.30        | 1.24     |
| 41  | P     | 65  | ALA  | C-O   | 5.06  | 1.30        | 1.24     |
| 32  | G     | 216 | VAL  | C-O   | 5.04  | 1.29        | 1.24     |
| 40  | O     | 47  | GLU  | C-O   | 5.04  | 1.29        | 1.23     |
| 52  | a     | 222 | VAL  | C-O   | 5.04  | 1.29        | 1.24     |
| 8   | i     | 55  | PRO  | C-O   | 5.03  | 1.30        | 1.24     |
| 52  | a     | 183 | ASP  | C-O   | 5.03  | 1.30        | 1.24     |
| 34  | I     | 154 | VAL  | C-O   | 5.02  | 1.30        | 1.24     |
| 59  | 8     | 94  | ASP  | C-O   | -5.02 | 1.17        | 1.24     |
| 4   | e     | 52  | ALA  | C-O   | 5.02  | 1.29        | 1.24     |
| 12  | m     | 118 | LYS  | C-O   | 5.01  | 1.30        | 1.24     |
| 18  | s     | 45  | VAL  | N-CA  | 5.00  | 1.52        | 1.46     |

All (578) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 48  | W     | 12   | PHE  | CA-C-O      | 14.32  | 130.50      | 120.19   |
| 34  | I     | 154  | VAL  | CA-C-N      | -13.81 | 100.68      | 120.29   |
| 34  | I     | 154  | VAL  | C-N-CA      | -13.81 | 100.68      | 120.29   |
| 59  | 8     | 86   | ILE  | N-CA-C      | 11.72  | 124.69      | 106.88   |
| 43  | R     | 96   | VAL  | N-CA-C      | 11.38  | 124.14      | 113.10   |
| 18  | s     | 35   | ILE  | N-CA-C      | -11.15 | 101.81      | 112.96   |
| 21  | v     | 91   | PHE  | CA-C-N      | -11.06 | 108.54      | 122.37   |
| 21  | v     | 91   | PHE  | C-N-CA      | -11.06 | 108.54      | 122.37   |
| 52  | a     | 164  | ARG  | CA-C-N      | -10.82 | 100.88      | 121.54   |
| 52  | a     | 164  | ARG  | C-N-CA      | -10.82 | 100.88      | 121.54   |
| 40  | O     | 44   | THR  | N-CA-C      | 10.67  | 124.96      | 110.55   |
| 40  | O     | 39   | PRO  | CA-C-N      | -10.62 | 102.48      | 122.13   |
| 40  | O     | 39   | PRO  | C-N-CA      | -10.62 | 102.48      | 122.13   |
| 39  | N     | 14   | SER  | CA-C-N      | -10.11 | 109.05      | 123.00   |
| 39  | N     | 14   | SER  | C-N-CA      | -10.11 | 109.05      | 123.00   |
| 52  | a     | 198  | LYS  | CA-C-N      | -10.10 | 107.28      | 122.83   |
| 52  | a     | 198  | LYS  | C-N-CA      | -10.10 | 107.28      | 122.83   |
| 59  | 8     | 109  | ALA  | CA-C-N      | -10.07 | 110.27      | 123.17   |
| 59  | 8     | 109  | ALA  | C-N-CA      | -10.07 | 110.27      | 123.17   |
| 34  | I     | 184  | LYS  | N-CA-C      | 10.06  | 121.94      | 109.57   |
| 53  | 3     | 1061 | G    | C2'-C3'-O3' | 10.04  | 128.75      | 113.70   |
| 33  | H     | 147  | GLY  | CA-C-N      | -9.88  | 109.57      | 122.51   |
| 33  | H     | 147  | GLY  | C-N-CA      | -9.88  | 109.57      | 122.51   |
| 6   | g     | 41   | LYS  | O-C-N       | -9.84  | 109.51      | 122.59   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 8   | i     | 57  | VAL  | CA-C-N | -9.64 | 110.28      | 122.43   |
| 8   | i     | 57  | VAL  | C-N-CA | -9.64 | 110.28      | 122.43   |
| 59  | 8     | 91  | GLY  | N-CA-C | 9.61  | 122.88      | 111.35   |
| 8   | i     | 9   | LYS  | CA-C-N | -9.56 | 104.49      | 122.08   |
| 8   | i     | 9   | LYS  | C-N-CA | -9.56 | 104.49      | 122.08   |
| 52  | a     | 56  | ASP  | CA-C-N | -9.56 | 108.93      | 123.17   |
| 52  | a     | 56  | ASP  | C-N-CA | -9.56 | 108.93      | 123.17   |
| 52  | a     | 200 | LYS  | N-CA-C | 9.55  | 121.32      | 109.57   |
| 40  | O     | 29  | ALA  | N-CA-C | -9.55 | 103.73      | 114.62   |
| 41  | P     | 29  | THR  | CA-C-O | 9.50  | 131.57      | 119.98   |
| 8   | i     | 32  | VAL  | N-CA-C | 9.46  | 122.25      | 108.53   |
| 40  | O     | 39  | PRO  | N-CA-C | 9.35  | 131.72      | 112.47   |
| 52  | a     | 59  | VAL  | CA-C-O | 9.28  | 128.48      | 120.22   |
| 6   | g     | 13  | GLY  | O-C-N  | -9.26 | 110.67      | 122.70   |
| 7   | h     | 16  | SER  | N-CA-C | -9.17 | 101.37      | 111.36   |
| 51  | Z     | 58  | LYS  | N-CA-C | -9.15 | 101.21      | 111.82   |
| 6   | g     | 44  | ILE  | CA-C-N | -9.09 | 108.27      | 120.54   |
| 6   | g     | 44  | ILE  | C-N-CA | -9.09 | 108.27      | 120.54   |
| 34  | I     | 152 | SER  | O-C-N  | -9.05 | 110.56      | 122.59   |
| 39  | N     | 33  | SER  | N-CA-C | 8.90  | 122.09      | 110.43   |
| 41  | P     | 73  | VAL  | N-CA-C | -8.82 | 104.31      | 112.43   |
| 26  | A     | 39  | LYS  | N-CA-C | -8.77 | 104.62      | 114.62   |
| 14  | o     | 79  | ALA  | CA-C-N | -8.74 | 109.08      | 120.44   |
| 14  | o     | 79  | ALA  | C-N-CA | -8.74 | 109.08      | 120.44   |
| 59  | 8     | 123 | SER  | N-CA-C | -8.74 | 102.06      | 112.89   |
| 41  | P     | 29  | THR  | O-C-N  | -8.70 | 112.47      | 123.26   |
| 8   | i     | 34  | ILE  | N-CA-C | 8.67  | 119.23      | 110.82   |
| 8   | i     | 58  | ILE  | O-C-N  | 8.67  | 133.52      | 122.77   |
| 18  | s     | 2   | GLU  | N-CA-C | 8.65  | 122.39      | 111.24   |
| 8   | i     | 7   | TYR  | CA-C-N | -8.64 | 109.79      | 122.58   |
| 8   | i     | 7   | TYR  | C-N-CA | -8.64 | 109.79      | 122.58   |
| 59  | 8     | 94  | ASP  | N-CA-C | -8.47 | 102.73      | 113.23   |
| 59  | 8     | 120 | GLN  | CA-C-O | 8.47  | 126.56      | 118.34   |
| 3   | d     | 165 | HIS  | N-CA-C | 8.46  | 120.13      | 111.07   |
| 12  | m     | 38  | ARG  | CA-C-N | -8.45 | 115.65      | 122.16   |
| 12  | m     | 38  | ARG  | C-N-CA | -8.45 | 115.65      | 122.16   |
| 4   | e     | 144 | LYS  | CA-C-N | -8.42 | 110.79      | 122.92   |
| 4   | e     | 144 | LYS  | C-N-CA | -8.42 | 110.79      | 122.92   |
| 59  | 8     | 584 | HIS  | CA-C-O | 8.36  | 130.53      | 120.92   |
| 48  | W     | 12  | PHE  | O-C-N  | -8.27 | 116.91      | 123.11   |
| 52  | a     | 162 | ARG  | CA-C-N | -8.27 | 108.32      | 121.87   |
| 52  | a     | 162 | ARG  | C-N-CA | -8.27 | 108.32      | 121.87   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 43  | R     | 93  | GLY  | N-CA-C | -8.24 | 103.80      | 115.43   |
| 35  | J     | 70  | MET  | N-CA-C | 8.24  | 120.55      | 110.41   |
| 8   | i     | 31  | GLY  | CA-C-N | -8.20 | 112.53      | 123.10   |
| 8   | i     | 31  | GLY  | C-N-CA | -8.20 | 112.53      | 123.10   |
| 59  | 8     | 584 | HIS  | O-C-N  | -8.18 | 113.67      | 123.16   |
| 38  | M     | 125 | ILE  | N-CA-C | 8.17  | 118.10      | 110.42   |
| 8   | i     | 55  | PRO  | CA-C-N | -8.13 | 111.14      | 122.69   |
| 8   | i     | 55  | PRO  | C-N-CA | -8.13 | 111.14      | 122.69   |
| 8   | i     | 43  | ALA  | CA-C-N | -8.11 | 109.57      | 121.98   |
| 8   | i     | 43  | ALA  | C-N-CA | -8.11 | 109.57      | 121.98   |
| 18  | s     | 40  | ASN  | N-CA-C | 8.03  | 123.19      | 108.58   |
| 10  | k     | 25  | LEU  | N-CA-C | 8.01  | 121.40      | 110.35   |
| 6   | g     | 8   | LYS  | CA-C-O | -8.00 | 109.07      | 120.51   |
| 39  | N     | 100 | ALA  | N-CA-C | -7.98 | 104.01      | 114.31   |
| 59  | 8     | 627 | ASN  | CA-C-N | -7.89 | 106.47      | 121.54   |
| 59  | 8     | 627 | ASN  | C-N-CA | -7.89 | 106.47      | 121.54   |
| 6   | g     | 145 | ASN  | CA-C-N | -7.88 | 112.88      | 123.12   |
| 6   | g     | 145 | ASN  | C-N-CA | -7.88 | 112.88      | 123.12   |
| 44  | S     | 47  | LEU  | CA-C-N | -7.88 | 110.05      | 122.65   |
| 44  | S     | 47  | LEU  | C-N-CA | -7.88 | 110.05      | 122.65   |
| 6   | g     | 45  | GLU  | N-CA-C | 7.83  | 120.50      | 111.11   |
| 11  | l     | 96  | LYS  | N-CA-C | -7.81 | 102.76      | 111.82   |
| 9   | j     | 81  | ILE  | N-CA-C | 7.79  | 125.53      | 109.34   |
| 6   | g     | 137 | GLU  | CA-C-O | 7.78  | 127.34      | 118.47   |
| 59  | 8     | 596 | ALA  | CA-C-N | -7.72 | 108.58      | 120.31   |
| 59  | 8     | 596 | ALA  | C-N-CA | -7.72 | 108.58      | 120.31   |
| 8   | i     | 11  | GLN  | CA-C-N | 7.71  | 135.85      | 121.97   |
| 8   | i     | 11  | GLN  | C-N-CA | 7.71  | 135.85      | 121.97   |
| 59  | 8     | 102 | SER  | CA-C-N | -7.66 | 107.67      | 120.68   |
| 59  | 8     | 102 | SER  | C-N-CA | -7.66 | 107.67      | 120.68   |
| 41  | P     | 29  | THR  | CA-C-N | -7.63 | 113.86      | 122.48   |
| 41  | P     | 29  | THR  | C-N-CA | -7.63 | 113.86      | 122.48   |
| 21  | v     | 90  | ASP  | CA-C-O | 7.62  | 128.73      | 120.43   |
| 51  | Z     | 31  | VAL  | N-CA-C | -7.58 | 105.17      | 111.91   |
| 43  | R     | 99  | GLN  | N-CA-C | 7.57  | 118.68      | 108.23   |
| 59  | 8     | 474 | LYS  | O-C-N  | 7.55  | 129.85      | 122.07   |
| 50  | Y     | 65  | LEU  | CA-C-N | -7.50 | 111.64      | 122.45   |
| 50  | Y     | 65  | LEU  | C-N-CA | -7.50 | 111.64      | 122.45   |
| 7   | h     | 77  | VAL  | CA-C-N | -7.47 | 110.14      | 121.87   |
| 7   | h     | 77  | VAL  | C-N-CA | -7.47 | 110.14      | 121.87   |
| 6   | g     | 43  | ASN  | CA-C-N | -7.47 | 108.60      | 120.55   |
| 6   | g     | 43  | ASN  | C-N-CA | -7.47 | 108.60      | 120.55   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | i     | 27  | LEU  | CA-C-O      | 7.45  | 127.10      | 118.90   |
| 48  | W     | 55  | ALA  | CA-C-N      | -7.45 | 109.71      | 120.29   |
| 48  | W     | 55  | ALA  | C-N-CA      | -7.45 | 109.71      | 120.29   |
| 33  | H     | 57  | GLU  | CA-C-N      | -7.45 | 114.66      | 122.85   |
| 33  | H     | 57  | GLU  | C-N-CA      | -7.45 | 114.66      | 122.85   |
| 40  | O     | 73  | LEU  | O-C-N       | 7.41  | 134.22      | 122.96   |
| 55  | 2     | 119 | A    | N9-C1'-C2'  | 7.37  | 123.06      | 112.00   |
| 23  | x     | 46  | VAL  | CA-C-O      | 7.33  | 127.49      | 120.31   |
| 43  | R     | 99  | GLN  | CA-C-O      | 7.28  | 127.62      | 120.56   |
| 59  | 8     | 477 | PHE  | CA-C-N      | -7.28 | 112.15      | 122.63   |
| 59  | 8     | 477 | PHE  | C-N-CA      | -7.28 | 112.15      | 122.63   |
| 51  | Z     | 10  | PRO  | CA-C-N      | -7.25 | 111.00      | 122.17   |
| 51  | Z     | 10  | PRO  | C-N-CA      | -7.25 | 111.00      | 122.17   |
| 7   | h     | 18  | VAL  | CA-C-N      | -7.20 | 109.36      | 120.31   |
| 7   | h     | 18  | VAL  | C-N-CA      | -7.20 | 109.36      | 120.31   |
| 52  | a     | 184 | LYS  | CA-C-N      | -7.20 | 107.53      | 121.58   |
| 52  | a     | 184 | LYS  | C-N-CA      | -7.20 | 107.53      | 121.58   |
| 35  | J     | 111 | ARG  | CA-C-N      | -7.17 | 108.73      | 120.71   |
| 35  | J     | 111 | ARG  | C-N-CA      | -7.17 | 108.73      | 120.71   |
| 52  | a     | 174 | THR  | CA-C-N      | -7.17 | 113.32      | 121.85   |
| 52  | a     | 174 | THR  | C-N-CA      | -7.17 | 113.32      | 121.85   |
| 8   | i     | 15  | GLY  | CA-C-N      | -7.16 | 111.45      | 122.62   |
| 8   | i     | 15  | GLY  | C-N-CA      | -7.16 | 111.45      | 122.62   |
| 37  | L     | 44  | SER  | N-CA-C      | -7.13 | 103.55      | 111.82   |
| 36  | K     | 49  | TYR  | CA-C-O      | 7.09  | 126.64      | 119.76   |
| 18  | s     | 106 | VAL  | CA-C-N      | -7.07 | 113.88      | 123.14   |
| 18  | s     | 106 | VAL  | C-N-CA      | -7.07 | 113.88      | 123.14   |
| 56  | 5     | 2   | G    | C2'-C3'-O3' | 7.05  | 120.08      | 109.50   |
| 59  | 8     | 653 | LYS  | CA-C-N      | -7.03 | 113.35      | 123.06   |
| 59  | 8     | 653 | LYS  | C-N-CA      | -7.03 | 113.35      | 123.06   |
| 13  | n     | 4   | ARG  | CA-C-N      | -7.03 | 112.74      | 122.93   |
| 13  | n     | 4   | ARG  | C-N-CA      | -7.03 | 112.74      | 122.93   |
| 52  | a     | 45  | ALA  | CA-C-N      | -7.03 | 114.48      | 123.19   |
| 52  | a     | 45  | ALA  | C-N-CA      | -7.03 | 114.48      | 123.19   |
| 10  | k     | 112 | PHE  | CA-C-N      | -7.00 | 110.16      | 120.38   |
| 10  | k     | 112 | PHE  | C-N-CA      | -7.00 | 110.16      | 120.38   |
| 1   | b     | 12  | ARG  | N-CA-C      | -7.00 | 103.24      | 114.09   |
| 21  | v     | 90  | ASP  | O-C-N       | -6.98 | 115.38      | 123.27   |
| 59  | 8     | 587 | ASP  | N-CA-C      | -6.97 | 104.25      | 112.89   |
| 1   | b     | 262 | THR  | CA-C-N      | -6.96 | 109.47      | 120.60   |
| 1   | b     | 262 | THR  | C-N-CA      | -6.96 | 109.47      | 120.60   |
| 40  | O     | 83  | THR  | N-CA-C      | -6.95 | 104.43      | 113.12   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 59  | 8     | 628  | THR  | N-CA-C      | 6.93  | 125.57      | 110.80   |
| 6   | g     | 132  | PHE  | O-C-N       | 6.89  | 131.03      | 123.10   |
| 23  | x     | 49   | ARG  | CA-C-N      | -6.88 | 112.54      | 122.45   |
| 23  | x     | 49   | ARG  | C-N-CA      | -6.88 | 112.54      | 122.45   |
| 41  | P     | 19   | VAL  | CA-C-O      | 6.86  | 128.31      | 120.76   |
| 37  | L     | 104  | VAL  | CA-C-O      | 6.86  | 128.44      | 121.17   |
| 26  | A     | 18   | CYS  | N-CA-C      | -6.84 | 106.14      | 114.75   |
| 1   | b     | 203  | VAL  | O-C-N       | -6.83 | 115.66      | 122.97   |
| 13  | n     | 79   | LEU  | N-CA-C      | -6.82 | 102.02      | 110.41   |
| 21  | v     | 67   | GLY  | CA-C-O      | 6.81  | 126.57      | 119.01   |
| 16  | q     | 29   | ARG  | CA-C-O      | 6.80  | 127.73      | 119.64   |
| 17  | r     | 73   | LYS  | CA-C-N      | -6.79 | 113.88      | 123.11   |
| 17  | r     | 73   | LYS  | C-N-CA      | -6.79 | 113.88      | 123.11   |
| 40  | O     | 36   | VAL  | CA-C-N      | -6.77 | 108.62      | 121.54   |
| 40  | O     | 36   | VAL  | C-N-CA      | -6.77 | 108.62      | 121.54   |
| 53  | 3     | 1126 | U    | N1-C1'-C2'  | 6.76  | 122.14      | 112.00   |
| 54  | 1     | 477  | A    | N9-C1'-C2'  | 6.65  | 121.98      | 112.00   |
| 31  | F     | 21   | GLY  | N-CA-C      | -6.65 | 106.78      | 114.69   |
| 34  | I     | 138  | PRO  | CA-C-N      | -6.64 | 113.07      | 122.63   |
| 34  | I     | 138  | PRO  | C-N-CA      | -6.64 | 113.07      | 122.63   |
| 36  | K     | 13   | ASP  | CA-C-O      | 6.62  | 128.36      | 121.07   |
| 32  | G     | 206  | ILE  | CA-C-O      | 6.61  | 127.83      | 120.95   |
| 23  | x     | 22   | ASN  | CA-C-O      | 6.61  | 127.41      | 120.54   |
| 52  | a     | 60   | ARG  | CA-C-N      | -6.60 | 108.83      | 121.05   |
| 52  | a     | 60   | ARG  | C-N-CA      | -6.60 | 108.83      | 121.05   |
| 59  | 8     | 623  | THR  | CA-C-N      | 6.60  | 128.09      | 119.84   |
| 59  | 8     | 623  | THR  | C-N-CA      | 6.60  | 128.09      | 119.84   |
| 1   | b     | 49   | THR  | CA-C-N      | -6.60 | 113.68      | 122.99   |
| 1   | b     | 49   | THR  | C-N-CA      | -6.60 | 113.68      | 122.99   |
| 59  | 8     | 668  | THR  | CA-C-N      | -6.60 | 111.44      | 120.28   |
| 59  | 8     | 668  | THR  | C-N-CA      | -6.60 | 111.44      | 120.28   |
| 3   | d     | 119  | ILE  | CA-C-O      | 6.57  | 127.22      | 120.39   |
| 54  | 1     | 1130 | U    | C2'-C3'-O3' | 6.56  | 119.34      | 109.50   |
| 43  | R     | 109  | LYS  | CA-C-N      | -6.54 | 111.60      | 121.87   |
| 43  | R     | 109  | LYS  | C-N-CA      | -6.54 | 111.60      | 121.87   |
| 52  | a     | 212  | VAL  | CA-C-N      | -6.54 | 112.90      | 122.65   |
| 52  | a     | 212  | VAL  | C-N-CA      | -6.54 | 112.90      | 122.65   |
| 39  | N     | 31   | GLN  | O-C-N       | -6.53 | 113.90      | 122.59   |
| 8   | i     | 57   | VAL  | O-C-N       | 6.53  | 130.90      | 122.94   |
| 12  | m     | 99   | GLY  | CA-C-N      | -6.51 | 114.11      | 122.77   |
| 12  | m     | 99   | GLY  | C-N-CA      | -6.51 | 114.11      | 122.77   |
| 34  | I     | 184  | LYS  | CA-C-O      | 6.50  | 125.17      | 119.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32  | G     | 36   | LYS  | N-CA-C      | -6.50 | 103.63      | 113.51   |
| 32  | G     | 142  | LYS  | CA-C-N      | -6.49 | 111.07      | 120.29   |
| 32  | G     | 142  | LYS  | C-N-CA      | -6.49 | 111.07      | 120.29   |
| 23  | x     | 46   | VAL  | O-C-N       | -6.48 | 116.75      | 123.03   |
| 59  | 8     | 85   | ASN  | CA-C-O      | 6.44  | 127.80      | 120.84   |
| 16  | q     | 18   | LYS  | N-CA-C      | -6.44 | 105.43      | 113.55   |
| 54  | l     | 1020 | A    | C2'-C3'-O3' | 6.43  | 119.14      | 109.50   |
| 52  | a     | 195  | ALA  | CA-C-N      | -6.42 | 110.00      | 120.72   |
| 52  | a     | 195  | ALA  | C-N-CA      | -6.42 | 110.00      | 120.72   |
| 49  | X     | 38   | THR  | CA-C-N      | -6.42 | 114.02      | 122.94   |
| 49  | X     | 38   | THR  | C-N-CA      | -6.42 | 114.02      | 122.94   |
| 42  | Q     | 43   | LYS  | N-CA-C      | 6.41  | 123.98      | 109.81   |
| 43  | R     | 100  | ARG  | N-CA-C      | 6.40  | 124.44      | 110.80   |
| 4   | e     | 89   | THR  | CA-C-O      | 6.40  | 127.77      | 120.54   |
| 53  | 3     | 280  | C    | C2'-C3'-O3' | 6.40  | 119.10      | 109.50   |
| 18  | s     | 44   | ALA  | CA-C-N      | -6.37 | 112.54      | 120.56   |
| 18  | s     | 44   | ALA  | C-N-CA      | -6.37 | 112.54      | 120.56   |
| 14  | o     | 116  | GLN  | N-CA-C      | 6.35  | 118.30      | 109.15   |
| 59  | 8     | 120  | GLN  | O-C-N       | -6.35 | 114.74      | 120.71   |
| 41  | P     | 19   | VAL  | O-C-N       | -6.33 | 116.03      | 123.05   |
| 4   | e     | 8    | LYS  | CA-C-N      | -6.32 | 113.08      | 122.56   |
| 4   | e     | 8    | LYS  | C-N-CA      | -6.32 | 113.08      | 122.56   |
| 5   | f     | 111  | PRO  | CA-C-N      | -6.32 | 114.81      | 122.90   |
| 5   | f     | 111  | PRO  | C-N-CA      | -6.32 | 114.81      | 122.90   |
| 36  | K     | 42   | TRP  | CA-C-N      | -6.32 | 113.42      | 122.64   |
| 36  | K     | 42   | TRP  | C-N-CA      | -6.32 | 113.42      | 122.64   |
| 4   | e     | 89   | THR  | O-C-N       | -6.32 | 116.02      | 123.22   |
| 59  | 8     | 650  | THR  | CA-C-N      | -6.29 | 116.54      | 121.82   |
| 59  | 8     | 650  | THR  | C-N-CA      | -6.29 | 116.54      | 121.82   |
| 4   | e     | 144  | LYS  | N-CA-C      | -6.28 | 105.58      | 113.18   |
| 59  | 8     | 98   | GLU  | CA-C-N      | -6.28 | 112.65      | 120.56   |
| 59  | 8     | 98   | GLU  | C-N-CA      | -6.28 | 112.65      | 120.56   |
| 22  | w     | 60   | ASP  | CA-C-N      | -6.27 | 111.62      | 121.97   |
| 22  | w     | 60   | ASP  | C-N-CA      | -6.27 | 111.62      | 121.97   |
| 59  | 8     | 224  | GLU  | N-CA-C      | -6.27 | 104.45      | 111.28   |
| 35  | J     | 87   | VAL  | N-CA-C      | 6.26  | 122.37      | 109.34   |
| 43  | R     | 66   | GLY  | CA-C-O      | 6.25  | 127.49      | 121.05   |
| 32  | G     | 106  | VAL  | N-CA-C      | -6.25 | 103.82      | 112.50   |
| 38  | M     | 98   | LEU  | N-CA-C      | -6.25 | 105.56      | 113.43   |
| 53  | 3     | 1061 | G    | C3'-C2'-O2' | 6.24  | 120.07      | 110.70   |
| 32  | G     | 109  | SER  | N-CA-C      | -6.23 | 104.49      | 111.28   |
| 51  | Z     | 8    | ASN  | N-CA-C      | 6.23  | 124.07      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 39  | N     | 31   | GLN  | CA-C-O      | 6.22  | 129.40      | 120.51   |
| 48  | W     | 15   | GLU  | CA-C-N      | -6.17 | 109.31      | 121.41   |
| 48  | W     | 15   | GLU  | C-N-CA      | -6.17 | 109.31      | 121.41   |
| 59  | 8     | 239  | GLY  | N-CA-C      | -6.16 | 105.42      | 115.46   |
| 59  | 8     | 85   | ASN  | CA-C-N      | -6.14 | 115.33      | 122.95   |
| 59  | 8     | 85   | ASN  | C-N-CA      | -6.14 | 115.33      | 122.95   |
| 52  | a     | 164  | ARG  | O-C-N       | 6.14  | 130.76      | 123.33   |
| 59  | 8     | 53   | MET  | N-CA-C      | -6.13 | 103.74      | 110.91   |
| 6   | g     | 41   | LYS  | CA-C-O      | 6.11  | 129.25      | 120.51   |
| 8   | i     | 57   | VAL  | CA-C-O      | -6.11 | 113.50      | 120.65   |
| 6   | g     | 139  | PHE  | N-CA-C      | 6.08  | 119.47      | 109.85   |
| 12  | m     | 40   | ARG  | CA-C-N      | -6.08 | 114.53      | 123.05   |
| 12  | m     | 40   | ARG  | C-N-CA      | -6.08 | 114.53      | 123.05   |
| 52  | a     | 160  | GLN  | CA-C-N      | -6.08 | 114.05      | 122.69   |
| 52  | a     | 160  | GLN  | C-N-CA      | -6.08 | 114.05      | 122.69   |
| 22  | w     | 27   | VAL  | O-C-N       | 6.08  | 129.68      | 123.00   |
| 41  | P     | 102  | ALA  | CA-C-N      | -6.07 | 113.79      | 123.31   |
| 41  | P     | 102  | ALA  | C-N-CA      | -6.07 | 113.79      | 123.31   |
| 3   | d     | 51   | GLU  | CA-C-N      | -6.04 | 112.59      | 120.63   |
| 3   | d     | 51   | GLU  | C-N-CA      | -6.04 | 112.59      | 120.63   |
| 59  | 8     | 650  | THR  | CA-C-O      | 6.03  | 125.30      | 119.08   |
| 2   | c     | 180  | VAL  | N-CA-C      | 6.03  | 115.03      | 106.53   |
| 50  | Y     | 60   | GLN  | CA-C-N      | -6.01 | 112.71      | 120.65   |
| 50  | Y     | 60   | GLN  | C-N-CA      | -6.01 | 112.71      | 120.65   |
| 43  | R     | 7    | ASN  | N-CA-C      | 6.01  | 119.19      | 110.42   |
| 9   | j     | 80   | HIS  | CA-C-N      | -6.00 | 111.16      | 121.97   |
| 9   | j     | 80   | HIS  | C-N-CA      | -6.00 | 111.16      | 121.97   |
| 3   | d     | 119  | ILE  | O-C-N       | -6.00 | 116.84      | 123.20   |
| 13  | n     | 25   | ALA  | N-CA-C      | -5.99 | 104.83      | 111.36   |
| 2   | c     | 158  | GLY  | CA-C-O      | 5.99  | 125.66      | 119.01   |
| 39  | N     | 90   | ASP  | N-CA-C      | 5.96  | 123.50      | 110.80   |
| 24  | y     | 22   | LEU  | CA-C-N      | -5.95 | 110.17      | 121.54   |
| 24  | y     | 22   | LEU  | C-N-CA      | -5.95 | 110.17      | 121.54   |
| 4   | e     | 12   | VAL  | N-CA-C      | 5.95  | 116.42      | 110.23   |
| 33  | H     | 200  | TRP  | CA-C-N      | -5.94 | 115.03      | 123.11   |
| 33  | H     | 200  | TRP  | C-N-CA      | -5.94 | 115.03      | 123.11   |
| 35  | J     | 55   | VAL  | CB-CA-C     | -5.94 | 108.06      | 113.70   |
| 59  | 8     | 120  | GLN  | CA-C-N      | -5.93 | 112.43      | 119.84   |
| 59  | 8     | 120  | GLN  | C-N-CA      | -5.93 | 112.43      | 119.84   |
| 59  | 8     | 226  | ALA  | CA-C-N      | -5.93 | 113.03      | 121.33   |
| 59  | 8     | 226  | ALA  | C-N-CA      | -5.93 | 113.03      | 121.33   |
| 53  | 3     | 1168 | U    | O4'-C4'-C3' | -5.92 | 98.08       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12  | m     | 40   | ARG  | CA-C-O      | 5.91  | 127.19      | 119.98   |
| 9   | j     | 40   | HIS  | N-CA-C      | -5.90 | 107.32      | 114.75   |
| 38  | M     | 38   | VAL  | CA-C-N      | -5.89 | 112.78      | 120.44   |
| 38  | M     | 38   | VAL  | C-N-CA      | -5.89 | 112.78      | 120.44   |
| 36  | K     | 66   | ALA  | N-CA-C      | 5.89  | 113.31      | 108.07   |
| 51  | Z     | 11   | PHE  | N-CA-C      | 5.88  | 120.00      | 112.12   |
| 59  | 8     | 421  | GLU  | CA-C-O      | 5.88  | 125.15      | 119.62   |
| 8   | i     | 32   | VAL  | O-C-N       | -5.88 | 117.14      | 123.14   |
| 59  | 8     | 228  | GLU  | CA-C-O      | 5.88  | 125.25      | 118.55   |
| 59  | 8     | 228  | GLU  | O-C-N       | -5.88 | 115.87      | 122.10   |
| 7   | h     | 63   | ALA  | CA-C-N      | -5.88 | 112.08      | 120.42   |
| 7   | h     | 63   | ALA  | C-N-CA      | -5.88 | 112.08      | 120.42   |
| 46  | U     | 54   | LEU  | N-CA-C      | 5.87  | 118.47      | 111.71   |
| 3   | d     | 194  | LYS  | CA-C-N      | -5.86 | 112.43      | 120.28   |
| 3   | d     | 194  | LYS  | C-N-CA      | -5.86 | 112.43      | 120.28   |
| 50  | Y     | 66   | ILE  | N-CA-C      | 5.85  | 118.26      | 109.20   |
| 4   | e     | 134  | GLN  | N-CA-C      | 5.84  | 120.69      | 113.50   |
| 52  | a     | 14   | LYS  | CA-C-N      | -5.84 | 113.94      | 122.58   |
| 52  | a     | 14   | LYS  | C-N-CA      | -5.84 | 113.94      | 122.58   |
| 52  | a     | 199  | ALA  | N-CA-C      | -5.83 | 105.98      | 112.57   |
| 53  | 3     | 1158 | C    | N1-C1'-C2'  | 5.83  | 120.75      | 112.00   |
| 6   | g     | 38   | PRO  | CA-C-O      | 5.81  | 127.96      | 121.34   |
| 24  | y     | 40   | SER  | CA-C-O      | 5.80  | 126.51      | 119.38   |
| 10  | k     | 106  | GLU  | CA-C-N      | -5.79 | 112.96      | 121.99   |
| 10  | k     | 106  | GLU  | C-N-CA      | -5.79 | 112.96      | 121.99   |
| 32  | G     | 50   | ASN  | N-CA-C      | -5.79 | 104.88      | 111.07   |
| 1   | b     | 132  | ARG  | N-CA-C      | -5.78 | 105.61      | 114.16   |
| 2   | c     | 157  | LYS  | O-C-N       | 5.78  | 129.98      | 122.87   |
| 45  | T     | 37   | HIS  | N-CA-C      | -5.78 | 105.06      | 111.36   |
| 8   | i     | 58   | ILE  | CA-C-O      | -5.77 | 113.71      | 120.75   |
| 32  | G     | 141  | GLU  | CA-C-N      | -5.77 | 112.09      | 120.29   |
| 32  | G     | 141  | GLU  | C-N-CA      | -5.77 | 112.09      | 120.29   |
| 16  | q     | 31   | TYR  | N-CA-C      | 5.76  | 118.05      | 111.02   |
| 3   | d     | 166  | LYS  | CA-C-N      | -5.75 | 115.45      | 123.10   |
| 3   | d     | 166  | LYS  | C-N-CA      | -5.75 | 115.45      | 123.10   |
| 53  | 3     | 1183 | U    | C2'-C3'-O3' | -5.75 | 105.08      | 113.70   |
| 6   | g     | 132  | PHE  | CA-C-N      | -5.74 | 113.15      | 122.34   |
| 6   | g     | 132  | PHE  | C-N-CA      | -5.74 | 113.15      | 122.34   |
| 33  | H     | 45   | GLU  | N-CA-C      | -5.73 | 106.94      | 114.04   |
| 53  | 3     | 1164 | G    | C2'-C3'-O3' | 5.72  | 118.08      | 109.50   |
| 37  | L     | 143  | MET  | CA-C-N      | -5.72 | 111.60      | 121.66   |
| 37  | L     | 143  | MET  | C-N-CA      | -5.72 | 111.60      | 121.66   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 11  | l     | 95   | LEU  | N-CA-C     | -5.71 | 106.44      | 113.41   |
| 34  | I     | 155  | LYS  | CA-C-O     | 5.71  | 126.48      | 120.42   |
| 59  | 8     | 406  | LEU  | N-CA-C     | 5.71  | 118.34      | 110.35   |
| 43  | R     | 25   | GLY  | N-CA-C     | -5.70 | 104.94      | 112.81   |
| 59  | 8     | 665  | GLY  | CA-C-O     | 5.70  | 126.19      | 119.46   |
| 7   | h     | 44   | ALA  | N-CA-C     | -5.70 | 105.59      | 112.54   |
| 24  | y     | 43   | LEU  | CA-C-N     | -5.70 | 112.85      | 120.54   |
| 24  | y     | 43   | LEU  | C-N-CA     | -5.70 | 112.85      | 120.54   |
| 26  | A     | 63   | ARG  | N-CA-C     | -5.69 | 106.34      | 113.28   |
| 36  | K     | 33   | GLU  | CA-C-O     | 5.68  | 127.03      | 119.59   |
| 4   | e     | 149  | ARG  | CA-C-N     | -5.68 | 114.12      | 120.53   |
| 4   | e     | 149  | ARG  | C-N-CA     | -5.68 | 114.12      | 120.53   |
| 37  | L     | 107  | ALA  | CA-C-N     | -5.68 | 110.70      | 121.54   |
| 37  | L     | 107  | ALA  | C-N-CA     | -5.68 | 110.70      | 121.54   |
| 52  | a     | 213  | SER  | CA-C-N     | -5.67 | 113.72      | 122.68   |
| 52  | a     | 213  | SER  | C-N-CA     | -5.67 | 113.72      | 122.68   |
| 26  | A     | 28   | VAL  | N-CA-C     | -5.67 | 108.32      | 113.71   |
| 10  | k     | 61   | VAL  | CA-C-N     | -5.67 | 113.21      | 121.71   |
| 10  | k     | 61   | VAL  | C-N-CA     | -5.67 | 113.21      | 121.71   |
| 18  | s     | 81   | SER  | CA-C-N     | -5.67 | 112.05      | 120.94   |
| 18  | s     | 81   | SER  | C-N-CA     | -5.67 | 112.05      | 120.94   |
| 10  | k     | 17   | ARG  | CA-C-N     | -5.66 | 112.93      | 121.86   |
| 10  | k     | 17   | ARG  | C-N-CA     | -5.66 | 112.93      | 121.86   |
| 59  | 8     | 296  | ASN  | CA-C-N     | -5.64 | 117.81      | 122.16   |
| 59  | 8     | 296  | ASN  | C-N-CA     | -5.64 | 117.81      | 122.16   |
| 40  | O     | 48   | ARG  | CA-C-N     | -5.63 | 114.84      | 122.95   |
| 40  | O     | 48   | ARG  | C-N-CA     | -5.63 | 114.84      | 122.95   |
| 17  | r     | 73   | LYS  | CA-C-O     | 5.63  | 127.02      | 120.49   |
| 53  | 3     | 983  | A    | N9-C1'-C2' | 5.62  | 120.44      | 112.00   |
| 41  | P     | 19   | VAL  | N-CA-C     | 5.61  | 116.75      | 108.45   |
| 54  | 1     | 2501 | C    | N1-C1'-C2' | 5.60  | 120.40      | 112.00   |
| 4   | e     | 114  | ARG  | N-CA-C     | -5.60 | 105.56      | 112.72   |
| 36  | K     | 16   | GLU  | CA-C-N     | -5.60 | 111.37      | 120.72   |
| 36  | K     | 16   | GLU  | C-N-CA     | -5.60 | 111.37      | 120.72   |
| 2   | c     | 201  | LEU  | O-C-N      | -5.59 | 116.79      | 123.27   |
| 59  | 8     | 586  | VAL  | CA-C-N     | -5.59 | 111.36      | 121.14   |
| 59  | 8     | 586  | VAL  | C-N-CA     | -5.59 | 111.36      | 121.14   |
| 59  | 8     | 101  | ARG  | N-CA-C     | 5.58  | 117.06      | 110.97   |
| 5   | f     | 88   | LEU  | CA-C-N     | -5.58 | 115.81      | 122.22   |
| 5   | f     | 88   | LEU  | C-N-CA     | -5.58 | 115.81      | 122.22   |
| 6   | g     | 44   | ILE  | N-CA-C     | -5.57 | 104.92      | 111.00   |
| 1   | b     | 41   | GLY  | O-C-N      | 5.57  | 128.86      | 122.34   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | w     | 30   | GLY  | N-CA-C      | -5.56 | 107.69      | 114.92   |
| 38  | M     | 45   | ILE  | CA-C-O      | 5.56  | 127.17      | 121.28   |
| 54  | 1     | 2296 | U    | C4'-C3'-O3' | 5.55  | 117.73      | 109.40   |
| 6   | g     | 42   | LYS  | CA-C-N      | -5.55 | 111.73      | 120.60   |
| 6   | g     | 42   | LYS  | C-N-CA      | -5.55 | 111.73      | 120.60   |
| 51  | Z     | 9    | GLU  | CA-C-N      | -5.54 | 112.91      | 119.84   |
| 51  | Z     | 9    | GLU  | C-N-CA      | -5.54 | 112.91      | 119.84   |
| 54  | 1     | 1331 | G    | N9-C1'-C2'  | 5.54  | 120.31      | 112.00   |
| 32  | G     | 209  | VAL  | N-CA-C      | -5.53 | 105.14      | 110.72   |
| 35  | J     | 123  | LEU  | N-CA-C      | -5.53 | 101.46      | 110.20   |
| 52  | a     | 30   | LEU  | N-CA-C      | -5.53 | 105.80      | 112.54   |
| 3   | d     | 163  | ASN  | CA-C-O      | 5.52  | 124.77      | 118.47   |
| 53  | 3     | 1332 | A    | N9-C1'-C2'  | 5.52  | 120.28      | 112.00   |
| 47  | V     | 51   | GLU  | N-CA-C      | -5.52 | 104.39      | 113.50   |
| 26  | A     | 45   | THR  | CA-C-O      | 5.52  | 125.81      | 119.35   |
| 26  | A     | 51   | VAL  | N-CA-C      | 5.51  | 120.80      | 109.34   |
| 8   | i     | 56   | VAL  | O-C-N       | 5.50  | 129.24      | 123.02   |
| 52  | a     | 179  | ASP  | N-CA-C      | -5.50 | 106.35      | 113.16   |
| 34  | I     | 4    | LEU  | N-CA-C      | 5.48  | 119.14      | 111.90   |
| 54  | 1     | 2343 | U    | N1-C1'-C2'  | 5.48  | 120.22      | 112.00   |
| 54  | 1     | 1178 | C    | N1-C1'-C2'  | 5.48  | 120.22      | 112.00   |
| 32  | G     | 128  | LEU  | N-CA-C      | -5.48 | 104.78      | 112.12   |
| 6   | g     | 113  | SER  | N-CA-C      | -5.47 | 106.44      | 113.01   |
| 7   | h     | 25   | ALA  | O-C-N       | 5.46  | 129.48      | 123.25   |
| 54  | 1     | 2287 | A    | N9-C1'-C2'  | 5.46  | 120.20      | 112.00   |
| 12  | m     | 4    | PRO  | CA-C-O      | 5.46  | 127.08      | 121.23   |
| 51  | Z     | 43   | GLU  | N-CA-C      | -5.45 | 105.50      | 111.82   |
| 20  | u     | 75   | ALA  | N-CA-C      | -5.45 | 104.99      | 111.69   |
| 7   | h     | 53   | ARG  | N-CA-C      | 5.44  | 118.51      | 110.46   |
| 39  | N     | 113  | LYS  | N-CA-C      | -5.44 | 100.93      | 109.25   |
| 21  | v     | 40   | ILE  | N-CA-C      | 5.44  | 117.72      | 108.86   |
| 52  | a     | 45   | ALA  | CA-C-O      | 5.43  | 126.00      | 120.24   |
| 59  | 8     | 474  | LYS  | CA-C-O      | -5.43 | 115.11      | 120.82   |
| 28  | C     | 27   | ARG  | N-CA-C      | 5.43  | 116.88      | 111.07   |
| 37  | L     | 144  | ALA  | N-CA-C      | -5.43 | 106.50      | 113.23   |
| 7   | h     | 65   | GLU  | N-CA-C      | -5.43 | 106.25      | 112.92   |
| 3   | d     | 119  | ILE  | CA-C-N      | -5.42 | 116.46      | 123.19   |
| 3   | d     | 119  | ILE  | C-N-CA      | -5.42 | 116.46      | 123.19   |
| 6   | g     | 114  | GLU  | CA-C-O      | 5.42  | 124.93      | 118.69   |
| 9   | j     | 11   | VAL  | N-CA-C      | 5.42  | 116.25      | 108.93   |
| 53  | 3     | 1122 | U    | N1-C1'-C2'  | 5.42  | 120.13      | 112.00   |
| 54  | 1     | 669  | G    | N9-C1'-C2'  | 5.41  | 120.12      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 43  | R     | 9    | PRO  | N-CA-C      | 5.41  | 119.80      | 111.57   |
| 11  | l     | 16   | GLY  | O-C-N       | -5.41 | 115.67      | 122.70   |
| 55  | 2     | 66   | A    | C2'-C3'-O3' | -5.41 | 105.59      | 113.70   |
| 41  | P     | 17   | ASP  | CA-C-N      | -5.41 | 116.31      | 122.42   |
| 41  | P     | 17   | ASP  | C-N-CA      | -5.41 | 116.31      | 122.42   |
| 5   | f     | 163  | TYR  | N-CA-C      | -5.41 | 101.91      | 109.96   |
| 7   | h     | 62   | ARG  | N-CA-C      | -5.40 | 104.88      | 112.12   |
| 32  | G     | 198  | VAL  | N-CA-C      | 5.39  | 116.55      | 109.21   |
| 53  | 3     | 964  | A    | N9-C1'-C2'  | 5.39  | 120.08      | 112.00   |
| 37  | L     | 69   | ARG  | N-CA-C      | 5.39  | 116.48      | 109.64   |
| 59  | 8     | 178  | HIS  | CA-C-N      | -5.39 | 111.25      | 121.54   |
| 59  | 8     | 178  | HIS  | C-N-CA      | -5.39 | 111.25      | 121.54   |
| 6   | g     | 38   | PRO  | O-C-N       | -5.38 | 116.52      | 123.03   |
| 59  | 8     | 50   | MET  | N-CA-C      | 5.38  | 118.67      | 112.97   |
| 59  | 8     | 301  | ASP  | N-CA-C      | 5.37  | 119.79      | 107.48   |
| 59  | 8     | 192  | ASN  | CA-C-N      | -5.37 | 113.34      | 123.27   |
| 59  | 8     | 192  | ASN  | C-N-CA      | -5.37 | 113.34      | 123.27   |
| 35  | J     | 109  | ALA  | O-C-N       | -5.37 | 115.45      | 122.59   |
| 53  | 3     | 1061 | G    | O4'-C4'-C3' | -5.36 | 98.64       | 104.00   |
| 37  | L     | 131  | GLY  | N-CA-C      | 5.36  | 120.72      | 111.98   |
| 45  | T     | 43   | ALA  | N-CA-C      | -5.36 | 105.13      | 110.97   |
| 35  | J     | 111  | ARG  | N-CA-C      | -5.36 | 104.89      | 111.75   |
| 21  | v     | 91   | PHE  | CA-C-O      | 5.35  | 126.03      | 120.30   |
| 53  | 3     | 1125 | U    | N1-C1'-C2'  | 5.34  | 120.01      | 112.00   |
| 43  | R     | 92   | ARG  | CA-C-N      | -5.34 | 112.46      | 121.85   |
| 43  | R     | 92   | ARG  | C-N-CA      | -5.34 | 112.46      | 121.85   |
| 54  | 1     | 2832 | U    | N1-C1'-C2'  | 5.33  | 120.00      | 112.00   |
| 20  | u     | 7    | ASP  | CA-C-N      | -5.33 | 114.10      | 122.73   |
| 20  | u     | 7    | ASP  | C-N-CA      | -5.33 | 114.10      | 122.73   |
| 45  | T     | 19   | ASN  | CA-C-N      | -5.33 | 114.09      | 122.08   |
| 45  | T     | 19   | ASN  | C-N-CA      | -5.33 | 114.09      | 122.08   |
| 16  | q     | 7    | VAL  | N-CA-C      | 5.33  | 116.05      | 110.62   |
| 18  | s     | 38   | TYR  | CA-C-O      | 5.33  | 127.00      | 120.55   |
| 10  | k     | 36   | GLY  | CA-C-N      | -5.32 | 113.59      | 122.64   |
| 10  | k     | 36   | GLY  | C-N-CA      | -5.32 | 113.59      | 122.64   |
| 53  | 3     | 428  | G    | N9-C1'-C2'  | 5.32  | 121.99      | 114.00   |
| 17  | r     | 44   | GLY  | N-CA-C      | -5.32 | 106.27      | 113.24   |
| 34  | I     | 63   | ILE  | CA-C-N      | -5.32 | 113.77      | 122.54   |
| 34  | I     | 63   | ILE  | C-N-CA      | -5.32 | 113.77      | 122.54   |
| 26  | A     | 13   | THR  | CA-C-N      | -5.32 | 115.61      | 123.05   |
| 26  | A     | 13   | THR  | C-N-CA      | -5.32 | 115.61      | 123.05   |
| 40  | O     | 39   | PRO  | CA-C-O      | -5.31 | 110.93      | 120.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42  | Q     | 99   | GLY  | CA-C-N      | -5.31 | 115.30      | 122.95   |
| 42  | Q     | 99   | GLY  | C-N-CA      | -5.31 | 115.30      | 122.95   |
| 52  | a     | 165  | ASN  | N-CA-C      | 5.31  | 122.11      | 110.80   |
| 38  | M     | 123  | GLU  | CA-C-N      | -5.30 | 115.98      | 122.93   |
| 38  | M     | 123  | GLU  | C-N-CA      | -5.30 | 115.98      | 122.93   |
| 59  | 8     | 228  | GLU  | N-CA-C      | -5.30 | 107.83      | 114.56   |
| 34  | I     | 33   | ILE  | N-CA-C      | 5.30  | 117.09      | 109.51   |
| 17  | r     | 74   | ILE  | CA-C-N      | -5.29 | 115.91      | 123.11   |
| 17  | r     | 74   | ILE  | C-N-CA      | -5.29 | 115.91      | 123.11   |
| 54  | 1     | 2501 | C    | C4'-C3'-O3' | -5.29 | 105.06      | 113.00   |
| 6   | g     | 123  | ARG  | N-CA-C      | -5.29 | 107.36      | 112.97   |
| 7   | h     | 36   | ASP  | CA-C-N      | -5.29 | 113.20      | 120.28   |
| 7   | h     | 36   | ASP  | C-N-CA      | -5.29 | 113.20      | 120.28   |
| 59  | 8     | 90   | PRO  | CA-C-O      | 5.28  | 127.10      | 119.34   |
| 28  | C     | 28   | THR  | CA-C-N      | -5.28 | 116.67      | 123.16   |
| 28  | C     | 28   | THR  | C-N-CA      | -5.28 | 116.67      | 123.16   |
| 19  | t     | 8    | LEU  | N-CA-C      | 5.28  | 117.03      | 111.28   |
| 37  | L     | 68   | VAL  | CA-C-N      | -5.27 | 113.06      | 120.39   |
| 37  | L     | 68   | VAL  | C-N-CA      | -5.27 | 113.06      | 120.39   |
| 37  | L     | 147  | ASN  | CA-C-N      | -5.27 | 114.80      | 122.86   |
| 37  | L     | 147  | ASN  | C-N-CA      | -5.27 | 114.80      | 122.86   |
| 42  | Q     | 89   | LEU  | CA-C-O      | 5.27  | 123.98      | 119.71   |
| 53  | 3     | 1345 | U    | N1-C1'-C2'  | 5.27  | 119.91      | 112.00   |
| 8   | i     | 12   | VAL  | N-CA-C      | -5.27 | 98.39       | 109.34   |
| 17  | r     | 58   | VAL  | CA-C-O      | 5.26  | 125.94      | 120.36   |
| 51  | Z     | 57   | LYS  | CA-C-N      | -5.26 | 112.31      | 120.31   |
| 51  | Z     | 57   | LYS  | C-N-CA      | -5.26 | 112.31      | 120.31   |
| 53  | 3     | 439  | U    | N1-C1'-C2'  | 5.26  | 119.88      | 112.00   |
| 1   | b     | 84   | PRO  | N-CA-C      | 5.25  | 120.98      | 113.47   |
| 35  | J     | 55   | VAL  | N-CA-C      | 5.25  | 119.24      | 112.67   |
| 11  | l     | 139  | GLY  | N-CA-C      | -5.25 | 108.44      | 114.69   |
| 42  | Q     | 115  | LYS  | N-CA-C      | -5.25 | 103.60      | 110.53   |
| 36  | K     | 18   | VAL  | N-CA-C      | 5.25  | 120.22      | 108.88   |
| 7   | h     | 59   | LEU  | CA-C-O      | 5.25  | 126.92      | 121.15   |
| 59  | 8     | 340  | SER  | CA-C-N      | -5.25 | 113.83      | 121.44   |
| 59  | 8     | 340  | SER  | C-N-CA      | -5.25 | 113.83      | 121.44   |
| 37  | L     | 49   | LEU  | N-CA-C      | -5.24 | 106.82      | 113.43   |
| 35  | J     | 125  | LYS  | CA-C-O      | 5.24  | 126.68      | 120.66   |
| 54  | 1     | 894  | U    | N1-C1'-C2'  | 5.24  | 119.85      | 112.00   |
| 16  | q     | 29   | ARG  | CA-C-N      | -5.23 | 115.43      | 122.91   |
| 16  | q     | 29   | ARG  | C-N-CA      | -5.23 | 115.43      | 122.91   |
| 52  | a     | 58   | ASN  | N-CA-C      | 5.23  | 117.08      | 110.33   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 59  | 8     | 421  | GLU  | CA-C-N     | -5.23 | 114.57      | 119.85   |
| 59  | 8     | 421  | GLU  | C-N-CA     | -5.23 | 114.57      | 119.85   |
| 40  | O     | 46   | LYS  | N-CA-C     | 5.22  | 118.24      | 110.14   |
| 3   | d     | 12   | LEU  | CA-C-O     | 5.22  | 126.24      | 120.71   |
| 54  | 1     | 1818 | U    | N1-C1'-C2' | 5.22  | 119.83      | 112.00   |
| 53  | 3     | 413  | G    | N9-C1'-C2' | 5.21  | 119.82      | 112.00   |
| 54  | 1     | 158  | U    | N1-C1'-C2' | 5.21  | 119.81      | 112.00   |
| 2   | c     | 202  | ILE  | CA-C-N     | -5.20 | 114.18      | 122.50   |
| 2   | c     | 202  | ILE  | C-N-CA     | -5.20 | 114.18      | 122.50   |
| 2   | c     | 146  | ILE  | N-CA-C     | 5.20  | 116.11      | 111.90   |
| 53  | 3     | 496  | A    | N9-C1'-C2' | 5.19  | 119.79      | 112.00   |
| 59  | 8     | 585  | ASP  | CA-C-N     | 5.19  | 131.31      | 121.97   |
| 59  | 8     | 585  | ASP  | C-N-CA     | 5.19  | 131.31      | 121.97   |
| 43  | R     | 56   | ARG  | CA-C-N     | -5.19 | 111.86      | 120.68   |
| 43  | R     | 56   | ARG  | C-N-CA     | -5.19 | 111.86      | 120.68   |
| 37  | L     | 86   | VAL  | CA-C-N     | -5.19 | 114.61      | 119.85   |
| 37  | L     | 86   | VAL  | C-N-CA     | -5.19 | 114.61      | 119.85   |
| 54  | 1     | 748  | G    | N9-C1'-C2' | 5.18  | 119.78      | 112.00   |
| 59  | 8     | 400  | PRO  | N-CA-C     | 5.18  | 123.14      | 112.47   |
| 14  | o     | 80   | GLU  | CA-C-N     | -5.18 | 112.44      | 120.31   |
| 14  | o     | 80   | GLU  | C-N-CA     | -5.18 | 112.44      | 120.31   |
| 34  | I     | 160  | LEU  | CA-C-N     | -5.18 | 112.07      | 120.72   |
| 34  | I     | 160  | LEU  | C-N-CA     | -5.18 | 112.07      | 120.72   |
| 9   | j     | 105  | VAL  | N-CA-C     | -5.17 | 107.78      | 112.12   |
| 1   | b     | 30   | ALA  | N-CA-C     | 5.17  | 121.23      | 109.81   |
| 59  | 8     | 122  | GLN  | CA-C-N     | -5.17 | 112.10      | 121.14   |
| 59  | 8     | 122  | GLN  | C-N-CA     | -5.17 | 112.10      | 121.14   |
| 5   | f     | 44   | HIS  | N-CA-C     | -5.16 | 103.05      | 111.04   |
| 8   | i     | 32   | VAL  | CA-C-O     | 5.15  | 126.59      | 120.72   |
| 35  | J     | 38   | VAL  | CA-C-N     | -5.15 | 114.47      | 121.27   |
| 35  | J     | 38   | VAL  | C-N-CA     | -5.15 | 114.47      | 121.27   |
| 17  | r     | 75   | VAL  | N-CA-C     | 5.14  | 114.98      | 107.37   |
| 18  | s     | 20   | VAL  | N-CA-C     | 5.14  | 115.81      | 110.82   |
| 1   | b     | 108  | GLY  | CA-C-N     | -5.14 | 114.94      | 122.19   |
| 1   | b     | 108  | GLY  | C-N-CA     | -5.14 | 114.94      | 122.19   |
| 44  | S     | 45   | LEU  | CA-C-N     | -5.14 | 113.08      | 122.38   |
| 44  | S     | 45   | LEU  | C-N-CA     | -5.14 | 113.08      | 122.38   |
| 48  | W     | 39   | VAL  | N-CA-C     | 5.14  | 114.56      | 108.96   |
| 53  | 3     | 967  | C    | N1-C1'-C2' | 5.14  | 119.71      | 112.00   |
| 53  | 3     | 1301 | U    | N1-C1'-C2' | 5.12  | 119.69      | 112.00   |
| 54  | 1     | 1328 | A    | N9-C1'-C2' | 5.12  | 119.68      | 112.00   |
| 19  | t     | 7    | LEU  | CA-C-N     | -5.12 | 113.42      | 120.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19  | t     | 7    | LEU  | C-N-CA      | -5.12 | 113.42      | 120.28   |
| 38  | M     | 45   | ILE  | O-C-N       | -5.12 | 117.17      | 123.00   |
| 17  | r     | 50   | GLY  | N-CA-C      | -5.11 | 101.07      | 113.18   |
| 10  | k     | 41   | ILE  | N-CA-C      | 5.11  | 116.26      | 108.80   |
| 33  | H     | 164  | THR  | CA-C-N      | -5.11 | 114.24      | 122.82   |
| 33  | H     | 164  | THR  | C-N-CA      | -5.11 | 114.24      | 122.82   |
| 38  | M     | 35   | ILE  | CA-C-O      | 5.10  | 126.26      | 120.85   |
| 26  | A     | 48   | GLN  | CA-C-N      | -5.10 | 111.08      | 121.18   |
| 26  | A     | 48   | GLN  | C-N-CA      | -5.10 | 111.08      | 121.18   |
| 5   | f     | 45   | ALA  | N-CA-C      | 5.09  | 121.65      | 110.80   |
| 33  | H     | 151  | GLU  | CA-C-N      | -5.09 | 116.87      | 123.19   |
| 33  | H     | 151  | GLU  | C-N-CA      | -5.09 | 116.87      | 123.19   |
| 54  | l     | 2333 | A    | C2'-C3'-O3' | -5.09 | 106.07      | 113.70   |
| 16  | q     | 3    | VAL  | N-CA-C      | 5.09  | 113.70      | 106.53   |
| 7   | h     | 45   | GLY  | N-CA-C      | -5.09 | 106.26      | 112.77   |
| 39  | N     | 31   | GLN  | CA-C-N      | -5.08 | 115.32      | 122.94   |
| 39  | N     | 31   | GLN  | C-N-CA      | -5.08 | 115.32      | 122.94   |
| 47  | V     | 45   | VAL  | N-CA-C      | 5.08  | 117.07      | 109.20   |
| 12  | m     | 35   | ALA  | O-C-N       | 5.08  | 128.64      | 122.85   |
| 32  | G     | 189  | ASN  | CA-C-N      | -5.07 | 113.00      | 122.73   |
| 32  | G     | 189  | ASN  | C-N-CA      | -5.07 | 113.00      | 122.73   |
| 59  | 8     | 94   | ASP  | CA-C-O      | 5.06  | 125.19      | 119.27   |
| 5   | f     | 112  | VAL  | CA-C-O      | 5.06  | 126.11      | 120.59   |
| 52  | a     | 62   | ALA  | CA-C-N      | -5.06 | 114.73      | 122.87   |
| 52  | a     | 62   | ALA  | C-N-CA      | -5.06 | 114.73      | 122.87   |
| 12  | m     | 71   | LYS  | CA-C-O      | 5.06  | 124.40      | 119.55   |
| 33  | H     | 183  | TYR  | CA-C-N      | -5.05 | 114.07      | 122.11   |
| 33  | H     | 183  | TYR  | C-N-CA      | -5.05 | 114.07      | 122.11   |
| 29  | D     | 30   | VAL  | N-CA-C      | -5.05 | 105.62      | 110.72   |
| 59  | 8     | 100  | GLU  | CA-C-O      | 5.05  | 126.30      | 120.90   |
| 16  | q     | 116  | LEU  | N-CA-C      | -5.05 | 106.63      | 112.89   |
| 59  | 8     | 465  | HIS  | CA-C-N      | -5.04 | 113.13      | 120.29   |
| 59  | 8     | 465  | HIS  | C-N-CA      | -5.04 | 113.13      | 120.29   |
| 4   | e     | 170  | ALA  | CA-C-N      | -5.04 | 112.30      | 120.72   |
| 4   | e     | 170  | ALA  | C-N-CA      | -5.04 | 112.30      | 120.72   |
| 11  | l     | 97   | ALA  | N-CA-C      | -5.04 | 105.88      | 112.23   |
| 21  | v     | 67   | GLY  | O-C-N       | -5.04 | 116.55      | 122.50   |
| 8   | i     | 9    | LYS  | O-C-N       | 5.03  | 128.97      | 122.93   |
| 59  | 8     | 103  | MET  | N-CA-C      | -5.03 | 105.89      | 112.23   |
| 37  | L     | 129  | ASN  | N-CA-C      | 5.03  | 118.26      | 111.17   |
| 50  | Y     | 60   | GLN  | CA-C-O      | 5.03  | 125.75      | 119.97   |
| 13  | n     | 20   | MET  | CA-C-N      | -5.02 | 113.16      | 120.29   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 13  | n     | 20   | MET  | C-N-CA     | -5.02 | 113.16      | 120.29   |
| 53  | 3     | 1303 | C    | N1-C1'-C2' | 5.02  | 119.53      | 112.00   |
| 11  | l     | 30   | THR  | CB-CA-C    | -5.02 | 104.86      | 109.83   |
| 59  | 8     | 478  | ASN  | N-CA-C     | 5.01  | 118.05      | 111.28   |
| 59  | 8     | 443  | PRO  | N-CA-C     | 5.01  | 122.78      | 112.47   |
| 6   | g     | 45   | GLU  | CA-C-N     | -5.00 | 113.08      | 120.28   |
| 6   | g     | 45   | GLU  | C-N-CA     | -5.00 | 113.08      | 120.28   |
| 31  | F     | 21   | GLY  | CA-C-O     | 5.00  | 124.62      | 119.27   |

There are no chirality outliers.

All (96) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | 1     | 1028 | A    | Sidechain |
| 54  | 1     | 1125 | G    | Sidechain |
| 54  | 1     | 1171 | G    | Sidechain |
| 54  | 1     | 119  | A    | Sidechain |
| 54  | 1     | 1204 | A    | Sidechain |
| 54  | 1     | 1271 | G    | Sidechain |
| 54  | 1     | 1328 | A    | Sidechain |
| 54  | 1     | 1377 | G    | Sidechain |
| 54  | 1     | 1419 | A    | Sidechain |
| 54  | 1     | 1432 | G    | Sidechain |
| 54  | 1     | 1615 | C    | Sidechain |
| 54  | 1     | 1647 | U    | Sidechain |
| 54  | 1     | 1666 | G    | Sidechain |
| 54  | 1     | 1768 | C    | Sidechain |
| 54  | 1     | 1775 | U    | Sidechain |
| 54  | 1     | 1828 | G    | Sidechain |
| 54  | 1     | 1834 | U    | Sidechain |
| 54  | 1     | 1937 | A    | Sidechain |
| 54  | 1     | 196  | A    | Sidechain |
| 54  | 1     | 1996 | C    | Sidechain |
| 54  | 1     | 2050 | C    | Sidechain |
| 54  | 1     | 2061 | G    | Sidechain |
| 54  | 1     | 221  | A    | Sidechain |
| 54  | 1     | 2266 | A    | Sidechain |
| 54  | 1     | 2273 | A    | Sidechain |
| 54  | 1     | 232  | G    | Sidechain |
| 54  | 1     | 2444 | G    | Sidechain |
| 54  | 1     | 2447 | G    | Sidechain |
| 54  | 1     | 2501 | C    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 54  | 1     | 2529 | G    | Sidechain |
| 54  | 1     | 2532 | G    | Sidechain |
| 54  | 1     | 27   | G    | Sidechain |
| 54  | 1     | 2718 | G    | Sidechain |
| 54  | 1     | 2725 | A    | Sidechain |
| 54  | 1     | 2778 | A    | Sidechain |
| 54  | 1     | 2848 | G    | Sidechain |
| 54  | 1     | 307  | G    | Sidechain |
| 54  | 1     | 370  | G    | Sidechain |
| 54  | 1     | 446  | G    | Sidechain |
| 54  | 1     | 450  | G    | Sidechain |
| 54  | 1     | 476  | G    | Sidechain |
| 54  | 1     | 477  | A    | Sidechain |
| 54  | 1     | 500  | G    | Sidechain |
| 54  | 1     | 501  | A    | Sidechain |
| 54  | 1     | 506  | G    | Sidechain |
| 54  | 1     | 51   | G    | Sidechain |
| 54  | 1     | 512  | G    | Sidechain |
| 54  | 1     | 562  | U    | Sidechain |
| 54  | 1     | 586  | A    | Sidechain |
| 54  | 1     | 683  | U    | Sidechain |
| 54  | 1     | 726  | G    | Sidechain |
| 54  | 1     | 727  | A    | Sidechain |
| 54  | 1     | 757  | G    | Sidechain |
| 54  | 1     | 775  | G    | Sidechain |
| 54  | 1     | 800  | A    | Sidechain |
| 54  | 1     | 810  | U    | Sidechain |
| 54  | 1     | 895  | U    | Sidechain |
| 54  | 1     | 975  | A    | Sidechain |
| 54  | 1     | 989  | G    | Sidechain |
| 55  | 2     | 1    | U    | Sidechain |
| 55  | 2     | 119  | A    | Sidechain |
| 55  | 2     | 24   | G    | Sidechain |
| 53  | 3     | 1121 | U    | Sidechain |
| 53  | 3     | 1122 | U    | Sidechain |
| 53  | 3     | 1123 | U    | Sidechain |
| 53  | 3     | 1150 | A    | Sidechain |
| 53  | 3     | 1164 | G    | Sidechain |
| 53  | 3     | 1167 | A    | Sidechain |
| 53  | 3     | 1168 | U    | Sidechain |
| 53  | 3     | 1171 | A    | Sidechain |
| 53  | 3     | 1182 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 53  | 3     | 1307 | U    | Sidechain         |
| 53  | 3     | 1316 | G    | Sidechain         |
| 53  | 3     | 1332 | A    | Sidechain         |
| 53  | 3     | 1333 | A    | Sidechain         |
| 53  | 3     | 159  | G    | Sidechain         |
| 53  | 3     | 324  | G    | Sidechain         |
| 53  | 3     | 413  | G    | Sidechain         |
| 53  | 3     | 428  | G    | Sidechain         |
| 53  | 3     | 496  | A    | Sidechain         |
| 53  | 3     | 521  | G    | Sidechain         |
| 53  | 3     | 780  | A    | Sidechain         |
| 53  | 3     | 872  | A    | Sidechain         |
| 53  | 3     | 884  | U    | Sidechain         |
| 53  | 3     | 898  | G    | Sidechain         |
| 53  | 3     | 920  | U    | Sidechain         |
| 53  | 3     | 946  | A    | Sidechain         |
| 56  | 5     | 3    | G    | Sidechain         |
| 59  | 8     | 623  | THR  | Mainchain         |
| 59  | 8     | 627  | ASN  | Mainchain         |
| 34  | I     | 152  | SER  | Mainchain         |
| 35  | J     | 92   | ARG  | Mainchain         |
| 6   | g     | 13   | GLY  | Peptide,Mainchain |
| 6   | g     | 41   | LYS  | Mainchain         |
| 6   | g     | 8    | LYS  | Mainchain         |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | b     | 2083  | 0        | 2157     | 111     | 0            |
| 2   | c     | 1565  | 0        | 1616     | 73      | 0            |
| 3   | d     | 1552  | 0        | 1619     | 75      | 0            |
| 4   | e     | 1411  | 0        | 1447     | 96      | 0            |
| 5   | f     | 1323  | 0        | 1374     | 79      | 0            |
| 6   | g     | 936   | 0        | 961      | 42      | 0            |
| 7   | h     | 633   | 0        | 666      | 58      | 0            |
| 8   | i     | 551   | 0        | 577      | 55      | 0            |
| 9   | j     | 1129  | 0        | 1162     | 66      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | k     | 939   | 0        | 1012     | 67      | 0            |
| 11  | l     | 1045  | 0        | 1117     | 74      | 0            |
| 12  | m     | 1074  | 0        | 1157     | 47      | 0            |
| 13  | n     | 961   | 0        | 1000     | 67      | 0            |
| 14  | o     | 892   | 0        | 923      | 44      | 0            |
| 15  | p     | 917   | 0        | 965      | 73      | 0            |
| 16  | q     | 947   | 0        | 1022     | 40      | 0            |
| 17  | r     | 816   | 0        | 839      | 48      | 0            |
| 18  | s     | 857   | 0        | 922      | 36      | 0            |
| 19  | t     | 739   | 0        | 807      | 27      | 0            |
| 20  | u     | 780   | 0        | 834      | 45      | 0            |
| 21  | v     | 753   | 0        | 780      | 52      | 0            |
| 22  | w     | 575   | 0        | 592      | 43      | 0            |
| 23  | x     | 625   | 0        | 655      | 30      | 0            |
| 24  | y     | 509   | 0        | 543      | 25      | 0            |
| 25  | z     | 449   | 0        | 491      | 23      | 0            |
| 26  | A     | 523   | 0        | 524      | 47      | 0            |
| 27  | B     | 444   | 0        | 461      | 18      | 0            |
| 28  | C     | 410   | 0        | 440      | 15      | 0            |
| 29  | D     | 377   | 0        | 418      | 23      | 0            |
| 30  | E     | 504   | 0        | 574      | 35      | 0            |
| 31  | F     | 302   | 0        | 343      | 21      | 0            |
| 32  | G     | 1705  | 0        | 1732     | 134     | 0            |
| 33  | H     | 1625  | 0        | 1699     | 87      | 0            |
| 34  | I     | 1643  | 0        | 1710     | 119     | 0            |
| 35  | J     | 1157  | 0        | 1199     | 120     | 0            |
| 36  | K     | 818   | 0        | 808      | 75      | 0            |
| 37  | L     | 1182  | 0        | 1240     | 74      | 0            |
| 38  | M     | 979   | 0        | 1034     | 74      | 0            |
| 39  | N     | 1022  | 0        | 1070     | 74      | 0            |
| 40  | O     | 787   | 0        | 828      | 116     | 0            |
| 41  | P     | 870   | 0        | 878      | 69      | 0            |
| 42  | Q     | 955   | 0        | 1019     | 72      | 0            |
| 43  | R     | 884   | 0        | 944      | 112     | 0            |
| 44  | S     | 805   | 0        | 847      | 103     | 0            |
| 45  | T     | 714   | 0        | 737      | 44      | 0            |
| 46  | U     | 649   | 0        | 666      | 50      | 0            |
| 47  | V     | 649   | 0        | 691      | 48      | 0            |
| 48  | W     | 536   | 0        | 552      | 38      | 0            |
| 49  | X     | 638   | 0        | 665      | 75      | 0            |
| 50  | Y     | 665   | 0        | 714      | 50      | 0            |
| 51  | Z     | 545   | 0        | 579      | 73      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 52  | a     | 1027   | 0        | 1092     | 86      | 0            |
| 53  | 3     | 33012  | 0        | 16618    | 1120    | 0            |
| 54  | 1     | 62317  | 0        | 31346    | 1346    | 0            |
| 55  | 2     | 2568   | 0        | 1303     | 73      | 0            |
| 56  | 5     | 1647   | 0        | 831      | 37      | 0            |
| 57  | 6     | 1640   | 0        | 837      | 26      | 0            |
| 58  | 4     | 346    | 0        | 175      | 13      | 0            |
| 59  | 8     | 5312   | 0        | 5283     | 418     | 0            |
| 60  | 1     | 10     | 0        | 10       | 0       | 0            |
| 61  | 5     | 7      | 0        | 7        | 0       | 0            |
| 62  | 8     | 32     | 0        | 14       | 3       | 0            |
| 63  | 8     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 153368 | 0        | 105126   | 5696    | 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 22.

All (5696) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:1115:U:H2'   | 53:3:1116:U:H5''  | 1.27                     | 1.15              |
| 40:O:37:ARG:O     | 53:3:1123:U:H5''  | 1.52                     | 1.09              |
| 54:1:1702:G:H2'   | 54:1:1703:G:H5''  | 1.29                     | 1.08              |
| 54:1:1906:G:H2'   | 54:1:1907:G:H5''  | 1.30                     | 1.08              |
| 56:5:13:C:H2'     | 56:5:14:A:H5''    | 1.39                     | 1.03              |
| 59:8:11:ARG:HE    | 59:8:283:ILE:HA   | 1.20                     | 1.03              |
| 59:8:349:VAL:HA   | 59:8:399:ASP:HB3  | 1.42                     | 1.02              |
| 41:P:122:PRO:HB2  | 51:Z:33:ARG:HA    | 1.42                     | 1.02              |
| 53:3:1306:A:H61   | 53:3:1331:G:H1'   | 1.23                     | 1.01              |
| 32:G:99:MET:HA    | 32:G:106:VAL:HG21 | 1.39                     | 1.01              |
| 4:e:140:ILE:HA    | 4:e:144:LYS:HE2   | 1.42                     | 1.00              |
| 54:1:45:G:H5''    | 54:1:46:G:H5'     | 1.40                     | 1.00              |
| 3:d:97:ASN:HB2    | 3:d:100:MET:HG2   | 1.44                     | 0.99              |
| 53:3:1091:U:H3'   | 53:3:1092:A:H5''  | 1.45                     | 0.99              |
| 53:3:850:U:H2'    | 53:3:851:G:H5''   | 1.42                     | 0.98              |
| 35:J:92:ARG:HB2   | 35:J:127:TYR:HB2  | 1.45                     | 0.98              |
| 54:1:1141:U:H4'   | 54:1:1142:A:O4'   | 1.62                     | 0.98              |
| 57:6:34:C:H3'     | 57:6:35:A:H8      | 1.29                     | 0.98              |
| 53:3:1116:U:H1'   | 53:3:1185:G:N1    | 1.79                     | 0.97              |
| 58:4:18:G:H2'     | 58:4:19:C:H5''    | 1.45                     | 0.97              |
| 10:k:104:THR:HG22 | 10:k:106:GLU:H    | 1.29                     | 0.96              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:1148:U:H3'   | 53:3:1149:C:H4'   | 1.46                     | 0.96              |
| 39:N:20:ILE:HD11  | 39:N:60:LEU:HD22  | 1.47                     | 0.96              |
| 15:p:3:ILE:H      | 15:p:3:ILE:HD12   | 1.31                     | 0.95              |
| 34:I:161:ALA:HA   | 34:I:164:ARG:HE   | 1.30                     | 0.95              |
| 5:f:10:VAL:HG12   | 5:f:48:THR:HA     | 1.47                     | 0.95              |
| 21:v:72:VAL:HG12  | 21:v:93:ARG:HA    | 1.48                     | 0.95              |
| 8:i:9:LYS:HB2     | 54:1:1061:U:H5''  | 1.48                     | 0.95              |
| 59:8:585:ASP:O    | 59:8:587:ASP:N    | 1.98                     | 0.95              |
| 53:3:1332:A:H2'   | 53:3:1333:A:C8    | 2.02                     | 0.95              |
| 13:n:83:LEU:HD22  | 13:n:87:PHE:HE2   | 1.31                     | 0.95              |
| 32:G:33:ALA:HB3   | 32:G:37:VAL:HG13  | 1.50                     | 0.94              |
| 18:s:90:LYS:HB2   | 18:s:92:ARG:HH12  | 1.29                     | 0.94              |
| 59:8:121:PRO:O    | 59:8:123:SER:N    | 2.01                     | 0.94              |
| 53:3:1332:A:H2'   | 53:3:1333:A:H8    | 1.31                     | 0.94              |
| 54:1:2048:G:H2'   | 54:1:2049:G:H5''  | 1.50                     | 0.94              |
| 20:u:73:ASN:HD21  | 20:u:75:ALA:HB3   | 1.33                     | 0.93              |
| 44:S:8:ARG:HE     | 53:3:1217:C:H5''  | 1.33                     | 0.93              |
| 28:C:28:THR:HG23  | 28:C:29:LYS:HG2   | 1.47                     | 0.93              |
| 53:3:1033:G:H2'   | 53:3:1034:G:H5''  | 1.50                     | 0.93              |
| 54:1:2800:A:H3'   | 54:1:2801:G:H5'   | 1.50                     | 0.93              |
| 41:P:126:ARG:HH22 | 53:3:692:U:H5''   | 1.34                     | 0.93              |
| 55:2:3:C:H2'      | 55:2:4:C:H5''     | 1.49                     | 0.93              |
| 12:m:12:MET:HA    | 54:1:910:A:H62    | 1.31                     | 0.92              |
| 54:1:1936:A:H2    | 54:1:1943:U:H3    | 1.14                     | 0.92              |
| 34:I:59:LYS:HE3   | 34:I:194:ILE:HG22 | 1.50                     | 0.92              |
| 53:3:1164:G:H22   | 53:3:1171:A:H61   | 1.18                     | 0.92              |
| 4:e:3:LEU:HA      | 4:e:6:TYR:HB3     | 1.48                     | 0.92              |
| 53:3:1259:C:H3'   | 53:3:1260:G:H5''  | 1.50                     | 0.92              |
| 53:3:1323:G:H2'   | 53:3:1324:A:H8    | 1.33                     | 0.92              |
| 6:g:47:PHE:HA     | 6:g:51:ARG:HB2    | 1.49                     | 0.92              |
| 53:3:1502:A:H8    | 53:3:1505:G:H22   | 1.18                     | 0.92              |
| 40:O:41:PRO:HD3   | 53:3:1150:A:C2    | 2.04                     | 0.92              |
| 53:3:1323:G:H2'   | 53:3:1324:A:C8    | 2.05                     | 0.92              |
| 35:J:22:LYS:HB3   | 35:J:29:ILE:HB    | 1.51                     | 0.92              |
| 52:a:196:LEU:HD12 | 52:a:209:ILE:HD11 | 1.51                     | 0.92              |
| 7:h:41:LEU:HD21   | 7:h:54:VAL:HB     | 1.49                     | 0.92              |
| 33:H:39:ARG:HG3   | 33:H:54:ILE:HD11  | 1.50                     | 0.92              |
| 1:b:180:MET:HE1   | 1:b:268:ARG:HE    | 1.34                     | 0.92              |
| 56:5:26:A:N6      | 56:5:44:G:H1      | 1.69                     | 0.91              |
| 25:z:16:LEU:HD23  | 25:z:16:LEU:H     | 1.35                     | 0.91              |
| 32:G:153:MET:HE1  | 32:G:157:PRO:HG3  | 1.53                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 59:8:121:PRO:C    | 59:8:123:SER:H    | 1.78                     | 0.90              |
| 35:J:54:GLU:HG3   | 35:J:56:PRO:HD2   | 1.53                     | 0.90              |
| 8:i:20:SER:HB3    | 8:i:21:PRO:HD3    | 1.53                     | 0.90              |
| 15:p:59:THR:HG22  | 15:p:72:VAL:HG12  | 1.54                     | 0.90              |
| 10:k:104:THR:HG22 | 10:k:106:GLU:N    | 1.86                     | 0.90              |
| 26:A:53:THR:HG21  | 49:X:21:ALA:HA    | 1.51                     | 0.90              |
| 20:u:73:ASN:ND2   | 20:u:75:ALA:HB3   | 1.86                     | 0.90              |
| 37:L:22:LEU:HD12  | 37:L:25:PHE:HB3   | 1.52                     | 0.90              |
| 43:R:97:ARG:HB2   | 53:3:1307:U:C2    | 2.06                     | 0.90              |
| 54:1:742:A:H2'    | 54:1:743:A:H8     | 1.35                     | 0.90              |
| 55:2:118:C:H2'    | 55:2:119:A:H8     | 1.37                     | 0.89              |
| 3:d:30:GLN:HE22   | 54:1:659:G:H21    | 1.13                     | 0.89              |
| 53:3:1306:A:N6    | 53:3:1331:G:H1'   | 1.86                     | 0.89              |
| 16:q:69:ARG:HH22  | 16:q:74:SER:HA    | 1.38                     | 0.89              |
| 36:K:3:HIS:H      | 36:K:92:THR:HG22  | 1.36                     | 0.89              |
| 59:8:111:MET:HE1  | 59:8:137:ARG:HB2  | 1.53                     | 0.89              |
| 53:3:405:U:H3'    | 53:3:406:G:H5'    | 1.54                     | 0.89              |
| 40:O:73:LEU:HD11  | 53:3:1124:G:H5'   | 1.55                     | 0.89              |
| 8:i:6:ALA:HB3     | 8:i:60:VAL:HB     | 1.54                     | 0.89              |
| 29:D:3:ARG:HA     | 29:D:3:ARG:HE     | 1.38                     | 0.88              |
| 32:G:136:ARG:NH1  | 32:G:136:ARG:HB3  | 1.88                     | 0.88              |
| 40:O:41:PRO:HD3   | 53:3:1150:A:H2    | 1.37                     | 0.88              |
| 10:k:103:VAL:HG23 | 10:k:104:THR:H    | 1.36                     | 0.88              |
| 59:8:20:ASP:H     | 62:8:801:GCP:H3B1 | 1.37                     | 0.88              |
| 40:O:80:THR:HB    | 40:O:83:THR:HG23  | 1.55                     | 0.88              |
| 48:W:33:THR:HG22  | 48:W:37:LYS:H     | 1.35                     | 0.88              |
| 51:Z:48:LYS:HD3   | 53:3:723:U:H6     | 1.36                     | 0.88              |
| 53:3:866:C:H4'    | 53:3:919:A:H5'    | 1.53                     | 0.88              |
| 7:h:56:ARG:HE     | 7:h:83:ALA:HB2    | 1.36                     | 0.88              |
| 7:h:57:ASN:HB2    | 7:h:62:ARG:HD2    | 1.52                     | 0.88              |
| 59:8:13:ILE:HG22  | 59:8:108:GLY:HA3  | 1.56                     | 0.88              |
| 1:b:270:ARG:HB3   | 1:b:270:ARG:HH11  | 1.39                     | 0.88              |
| 53:3:1086:U:H2'   | 53:3:1087:G:H8    | 1.39                     | 0.88              |
| 54:1:742:A:H2'    | 54:1:743:A:C8     | 2.09                     | 0.88              |
| 7:h:53:ARG:HB3    | 54:1:1084:A:OP1   | 1.73                     | 0.88              |
| 20:u:39:ASN:HD22  | 20:u:62:ALA:HB3   | 1.36                     | 0.88              |
| 43:R:97:ARG:H     | 53:3:1307:U:C3'   | 1.85                     | 0.87              |
| 53:3:1522:U:H2'   | 53:3:1523:G:C8    | 2.09                     | 0.87              |
| 26:A:52:ALA:HA    | 49:X:27:LYS:HB2   | 1.54                     | 0.87              |
| 59:8:75:MET:HG3   | 59:8:79:TYR:HB2   | 1.54                     | 0.87              |
| 53:3:1218:C:H2'   | 53:3:1219:A:C8    | 2.09                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 58:4:17:U:H2'     | 58:4:18:G:C8      | 2.10                     | 0.87              |
| 8:i:12:VAL:HA     | 54:1:1061:U:H3    | 1.39                     | 0.86              |
| 53:3:950:U:H2'    | 53:3:951:G:H8     | 1.38                     | 0.86              |
| 54:1:704:G:H2'    | 54:1:726:G:H22    | 1.38                     | 0.86              |
| 49:X:5:LYS:HB2    | 53:3:1314:C:OP2   | 1.75                     | 0.86              |
| 59:8:53:MET:HE1   | 59:8:63:ILE:HD13  | 1.58                     | 0.86              |
| 5:f:94:ARG:H      | 5:f:105:SER:HB2   | 1.41                     | 0.86              |
| 53:3:1164:G:N2    | 53:3:1171:A:H61   | 1.72                     | 0.86              |
| 31:F:22:VAL:HG13  | 31:F:37:GLN:HB3   | 1.57                     | 0.85              |
| 37:L:112:ASP:HB3  | 37:L:117:LEU:HD23 | 1.56                     | 0.85              |
| 43:R:99:GLN:HG3   | 43:R:100:ARG:N    | 1.90                     | 0.85              |
| 51:Z:9:GLU:HB3    | 51:Z:10:PRO:HD3   | 1.57                     | 0.85              |
| 26:A:20:ASN:HD21  | 26:A:39:LYS:HD2   | 1.41                     | 0.85              |
| 52:a:30:LEU:HD12  | 52:a:33:LEU:HD12  | 1.57                     | 0.85              |
| 44:S:52:ARG:HH11  | 53:3:1317:C:H42   | 1.20                     | 0.85              |
| 54:1:1906:G:C2'   | 54:1:1907:G:H5''  | 2.06                     | 0.85              |
| 59:8:323:LYS:HB3  | 59:8:335:PHE:HB2  | 1.58                     | 0.85              |
| 46:U:22:ALA:HA    | 46:U:33:ILE:HD13  | 1.59                     | 0.85              |
| 53:3:531:U:H4'    | 53:3:532:A:H5'    | 1.58                     | 0.85              |
| 53:3:1130:A:H61   | 53:3:1144:G:H1'   | 1.41                     | 0.85              |
| 54:1:1702:G:C2'   | 54:1:1703:G:H5''  | 2.05                     | 0.85              |
| 38:M:95:MET:HB3   | 38:M:98:LEU:HG    | 1.58                     | 0.85              |
| 53:3:1122:U:H2'   | 53:3:1123:U:C5    | 2.10                     | 0.85              |
| 43:R:89:ARG:HD3   | 43:R:94:LEU:HB3   | 1.59                     | 0.84              |
| 11:l:23:ILE:H     | 11:l:23:ILE:HD12  | 1.39                     | 0.84              |
| 51:Z:32:ARG:HH11  | 51:Z:33:ARG:HG3   | 1.41                     | 0.84              |
| 32:G:136:ARG:HB3  | 32:G:136:ARG:HH11 | 1.41                     | 0.84              |
| 32:G:15:PHE:HA    | 32:G:42:LEU:HD21  | 1.59                     | 0.84              |
| 42:Q:109:ARG:HB2  | 42:Q:118:VAL:HG21 | 1.57                     | 0.84              |
| 59:8:351:ASN:HB3  | 59:8:356:ALA:HB3  | 1.59                     | 0.84              |
| 27:B:54:ILE:HG23  | 27:B:56:LYS:H     | 1.41                     | 0.84              |
| 32:G:108:GLN:HG3  | 32:G:112:ARG:HH12 | 1.43                     | 0.84              |
| 5:f:34:ARG:HH12   | 5:f:36:LEU:HD13   | 1.41                     | 0.84              |
| 34:I:100:VAL:HG21 | 34:I:136:VAL:HG21 | 1.58                     | 0.84              |
| 34:I:195:ASN:HD21 | 34:I:197:HIS:HB3  | 1.39                     | 0.84              |
| 53:3:1502:A:H5'   | 53:3:1504:G:N7    | 1.92                     | 0.84              |
| 32:G:131:LYS:HD3  | 32:G:131:LYS:N    | 1.92                     | 0.83              |
| 40:O:41:PRO:CD    | 53:3:1150:A:C2    | 2.61                     | 0.83              |
| 40:O:40:ILE:HG13  | 40:O:73:LEU:HD12  | 1.60                     | 0.83              |
| 35:J:133:ILE:H    | 35:J:133:ILE:HD12 | 1.43                     | 0.83              |
| 37:L:15:PRO:HG2   | 37:L:43:TYR:HE2   | 1.41                     | 0.83              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:e:149:ARG:HD3  | 4:e:149:ARG:H     | 1.42                     | 0.83              |
| 41:P:30:ILE:HB   | 41:P:45:THR:HG22  | 1.59                     | 0.83              |
| 49:X:53:GLY:HA3  | 53:3:1221:G:H4'   | 1.60                     | 0.83              |
| 54:1:1394:U:H4'  | 54:1:1603:A:H4'   | 1.61                     | 0.83              |
| 54:1:2297:A:N1   | 54:1:2321:U:H5    | 1.77                     | 0.83              |
| 59:8:288:SER:H   | 59:8:291:ASP:HB2  | 1.43                     | 0.83              |
| 43:R:97:ARG:N    | 53:3:1307:U:H2'   | 1.94                     | 0.82              |
| 46:U:76:LYS:HD2  | 46:U:80:LYS:HZ1   | 1.42                     | 0.82              |
| 23:x:16:ASN:HD21 | 23:x:26:ARG:HB3   | 1.43                     | 0.82              |
| 32:G:132:GLU:HA  | 32:G:135:MET:HE2  | 1.59                     | 0.82              |
| 52:a:23:ILE:H    | 52:a:23:ILE:HD12  | 1.44                     | 0.82              |
| 54:1:799:G:H5''  | 54:1:800:A:H2'    | 1.61                     | 0.82              |
| 31:F:23:ILE:H    | 31:F:23:ILE:HD12  | 1.42                     | 0.82              |
| 35:J:80:LEU:HD22 | 35:J:122:VAL:HG11 | 1.60                     | 0.82              |
| 32:G:170:ILE:H   | 32:G:170:ILE:HD12 | 1.44                     | 0.82              |
| 18:s:83:LYS:HG2  | 18:s:95:ARG:HH11  | 1.44                     | 0.82              |
| 53:3:33:A:H2'    | 53:3:34:C:C6      | 2.14                     | 0.82              |
| 53:3:1522:U:H2'  | 53:3:1523:G:H8    | 1.42                     | 0.82              |
| 17:r:22:LEU:HD12 | 17:r:94:THR:HB    | 1.62                     | 0.82              |
| 33:H:55:VAL:HB   | 33:H:66:THR:HB    | 1.60                     | 0.82              |
| 42:Q:78:VAL:O    | 42:Q:102:ASP:HB2  | 1.78                     | 0.82              |
| 53:3:966:G:H2'   | 53:3:967:C:H5'    | 1.59                     | 0.82              |
| 59:8:282:VAL:O   | 59:8:286:LEU:HB2  | 1.80                     | 0.82              |
| 3:d:30:GLN:NE2   | 54:1:659:G:H21    | 1.78                     | 0.81              |
| 4:e:33:ILE:HB    | 4:e:90:LEU:HB2    | 1.61                     | 0.81              |
| 11:l:47:ARG:HB3  | 11:l:47:ARG:HH21  | 1.45                     | 0.81              |
| 40:O:41:PRO:CD   | 53:3:1150:A:H2    | 1.94                     | 0.81              |
| 52:a:27:ILE:HD13 | 52:a:186:LYS:HB2  | 1.63                     | 0.81              |
| 53:3:950:U:H2'   | 53:3:951:G:C8     | 2.15                     | 0.81              |
| 59:8:359:ARG:HG2 | 59:8:360:PHE:H    | 1.45                     | 0.81              |
| 53:3:1079:G:O2'  | 53:3:1080:A:H5'   | 1.80                     | 0.81              |
| 41:P:108:ASN:HB3 | 51:Z:6:ARG:HD3    | 1.63                     | 0.81              |
| 53:3:1524:C:H2'  | 53:3:1525:G:C8    | 2.16                     | 0.81              |
| 58:4:19:C:H3'    | 58:4:20:C:H5'     | 1.63                     | 0.81              |
| 7:h:29:ASP:HB2   | 7:h:56:ARG:HH12   | 1.44                     | 0.81              |
| 53:3:850:U:C2'   | 53:3:851:G:H5''   | 2.09                     | 0.81              |
| 53:3:530:G:H3'   | 53:3:531:U:H5''   | 1.62                     | 0.81              |
| 27:B:10:SER:O    | 27:B:14:MET:HG3   | 1.79                     | 0.81              |
| 43:R:97:ARG:H    | 53:3:1307:U:C2'   | 1.94                     | 0.81              |
| 59:8:120:GLN:O   | 59:8:121:PRO:O    | 2.00                     | 0.81              |
| 53:3:1148:U:H3'  | 53:3:1149:C:C4'   | 2.10                     | 0.80              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:w:33:ILE:HG22 | 22:w:34:VAL:HG23  | 1.64                     | 0.80              |
| 30:E:41:ARG:HG3  | 30:E:44:ARG:HH12  | 1.45                     | 0.80              |
| 13:n:12:ARG:HD3  | 13:n:16:HIS:CE1   | 2.16                     | 0.80              |
| 32:G:35:ASN:HB3  | 32:G:37:VAL:HG12  | 1.63                     | 0.80              |
| 52:a:60:ARG:HE   | 52:a:164:ARG:HH11 | 1.28                     | 0.80              |
| 54:1:2121:G:H2'  | 54:1:2122:U:O4'   | 1.82                     | 0.80              |
| 34:I:96:ARG:HE   | 34:I:133:SER:HA   | 1.46                     | 0.80              |
| 49:X:9:PHE:CZ    | 53:3:1318:A:H4'   | 2.17                     | 0.80              |
| 40:O:57:VAL:HG22 | 40:O:58:ASN:H     | 1.44                     | 0.80              |
| 10:k:13:ASN:HD22 | 10:k:98:ARG:HB3   | 1.46                     | 0.80              |
| 40:O:52:LEU:HB2  | 44:S:80:ARG:HD2   | 1.62                     | 0.80              |
| 53:3:1225:A:H5'  | 53:3:1226:C:OP2   | 1.80                     | 0.80              |
| 5:f:97:VAL:HG23  | 5:f:124:CYS:SG    | 2.22                     | 0.80              |
| 35:J:10:LEU:HD12 | 35:J:11:GLN:N     | 1.97                     | 0.80              |
| 39:N:98:ARG:HG3  | 39:N:103:VAL:HG21 | 1.63                     | 0.80              |
| 52:a:15:VAL:HG11 | 52:a:220:ALA:HB3  | 1.64                     | 0.80              |
| 10:k:24:VAL:HG13 | 10:k:33:ALA:HB2   | 1.61                     | 0.79              |
| 59:8:362:ARG:H   | 59:8:362:ARG:HD3  | 1.47                     | 0.79              |
| 49:X:53:GLY:CA   | 53:3:1221:G:H4'   | 2.12                     | 0.79              |
| 53:3:1512:U:H2'  | 53:3:1513:A:C8    | 2.17                     | 0.79              |
| 40:O:37:ARG:O    | 53:3:1123:U:C5'   | 2.30                     | 0.79              |
| 56:5:13:C:C2'    | 56:5:14:A:H5''    | 2.12                     | 0.79              |
| 59:8:366:MET:HE1 | 59:8:371:ARG:HA   | 1.63                     | 0.79              |
| 24:y:17:GLU:HB3  | 24:y:53:VAL:HG11  | 1.64                     | 0.79              |
| 37:L:129:ASN:HA  | 37:L:134:VAL:HG11 | 1.64                     | 0.79              |
| 53:3:946:A:H61   | 53:3:1235:U:H3    | 1.29                     | 0.79              |
| 53:3:1061:G:H2'  | 53:3:1062:U:H4'   | 1.65                     | 0.79              |
| 37:L:14:ASP:HB2  | 37:L:19:SER:HB3   | 1.65                     | 0.79              |
| 53:3:1197:A:H2'  | 53:3:1198:G:H5''  | 1.63                     | 0.79              |
| 55:2:119:A:C2    | 55:2:120:A:H1'    | 2.16                     | 0.79              |
| 40:O:73:LEU:CD1  | 53:3:1124:G:H5'   | 2.13                     | 0.79              |
| 13:n:63:ARG:NH2  | 54:1:1454:C:H5'   | 1.97                     | 0.79              |
| 26:A:14:ALA:HB3  | 26:A:22:MET:O     | 1.82                     | 0.79              |
| 53:3:135:C:H2'   | 53:3:136:C:H5'    | 1.63                     | 0.79              |
| 53:3:1295:U:H2'  | 53:3:1296:C:C6    | 2.17                     | 0.79              |
| 15:p:38:ARG:HG2  | 15:p:39:LEU:H     | 1.48                     | 0.79              |
| 32:G:96:LEU:HD23 | 32:G:99:MET:HB3   | 1.64                     | 0.79              |
| 35:J:152:VAL:HA  | 35:J:155:LYS:HG2  | 1.65                     | 0.79              |
| 53:3:1060:U:H3   | 53:3:1197:A:H61   | 1.29                     | 0.79              |
| 20:u:39:ASN:ND2  | 20:u:62:ALA:HB3   | 1.97                     | 0.78              |
| 38:M:17:GLN:HE21 | 38:M:71:VAL:HB    | 1.45                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:H:123:LEU:HD21 | 33:H:129:PHE:HB3  | 1.64                     | 0.78              |
| 37:L:74:VAL:HG12  | 37:L:87:PRO:HA    | 1.62                     | 0.78              |
| 42:Q:72:ASN:H     | 42:Q:73:LEU:HD12  | 1.47                     | 0.78              |
| 54:1:1068:G:H21   | 54:1:1096:A:H5'   | 1.48                     | 0.78              |
| 34:I:150:LYS:HD3  | 34:I:177:MET:HE3  | 1.65                     | 0.78              |
| 53:3:976:G:H2'    | 53:3:1362:A:C2    | 2.18                     | 0.78              |
| 54:1:1181:U:H2'   | 54:1:1182:G:C8    | 2.18                     | 0.78              |
| 55:2:115:A:H2'    | 55:2:116:G:C8     | 2.18                     | 0.78              |
| 53:3:575:G:O2'    | 53:3:821:G:H5'    | 1.84                     | 0.78              |
| 54:1:593:U:H2'    | 54:1:594:U:C6     | 2.18                     | 0.78              |
| 9:j:16:TYR:O      | 9:j:55:ILE:HG22   | 1.83                     | 0.78              |
| 31:F:36:ARG:HD2   | 31:F:37:GLN:HG3   | 1.66                     | 0.78              |
| 49:X:35:ARG:CZ    | 49:X:74:ALA:HB3   | 2.13                     | 0.78              |
| 50:Y:80:ALA:HA    | 50:Y:83:ASN:HD21  | 1.46                     | 0.78              |
| 54:1:2553:G:H3'   | 54:1:2554:U:H5''  | 1.65                     | 0.78              |
| 32:G:129:THR:HB   | 32:G:131:LYS:HE2  | 1.63                     | 0.78              |
| 59:8:282:VAL:HG13 | 59:8:286:LEU:HD22 | 1.66                     | 0.78              |
| 34:I:149:LYS:HG2  | 34:I:150:LYS:HG2  | 1.66                     | 0.77              |
| 35:J:67:ARG:NH1   | 35:J:67:ARG:HB2   | 1.98                     | 0.77              |
| 36:K:11:HIS:ND1   | 36:K:12:PRO:HD2   | 1.99                     | 0.77              |
| 43:R:97:ARG:H     | 53:3:1307:U:H2'   | 1.49                     | 0.77              |
| 51:Z:48:LYS:HE3   | 53:3:724:G:OP1    | 1.84                     | 0.77              |
| 30:E:30:HIS:O     | 30:E:32:LEU:N     | 2.17                     | 0.77              |
| 37:L:50:ALA:HB2   | 37:L:57:GLU:HG3   | 1.67                     | 0.77              |
| 37:L:85:GLN:HB2   | 37:L:147:ASN:HB2  | 1.65                     | 0.77              |
| 8:i:13:ALA:HA     | 8:i:53:PRO:HA     | 1.67                     | 0.77              |
| 11:l:47:ARG:HB3   | 11:l:47:ARG:NH2   | 1.97                     | 0.77              |
| 41:P:53:GLY:O     | 41:P:56:LYS:HG2   | 1.84                     | 0.77              |
| 43:R:22:TYR:HD2   | 43:R:65:GLU:HA    | 1.50                     | 0.77              |
| 49:X:62:THR:HG22  | 49:X:65:MET:HE3   | 1.66                     | 0.77              |
| 54:1:1509:A:H2'   | 54:1:1510:G:C8    | 2.20                     | 0.77              |
| 59:8:473:MET:HB3  | 59:8:479:VAL:HB   | 1.66                     | 0.77              |
| 12:m:41:LEU:HD13  | 12:m:96:ILE:HG13  | 1.66                     | 0.77              |
| 53:3:1116:U:H1'   | 53:3:1185:G:H1    | 1.50                     | 0.77              |
| 57:6:34:C:H3'     | 57:6:35:A:C8      | 2.18                     | 0.77              |
| 58:4:18:G:C2'     | 58:4:19:C:H5''    | 2.15                     | 0.77              |
| 59:8:138:ILE:HD13 | 59:8:286:LEU:HD11 | 1.66                     | 0.77              |
| 59:8:445:PHE:HE1  | 59:8:458:ILE:HG23 | 1.50                     | 0.77              |
| 18:s:82:MET:HB3   | 18:s:84:ARG:HH22  | 1.50                     | 0.77              |
| 40:O:85:ASP:HB2   | 40:O:89:ARG:HH12  | 1.48                     | 0.77              |
| 43:R:51:GLN:HA    | 43:R:54:THR:HG23  | 1.64                     | 0.77              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 19:t:64:LYS:HE2  | 19:t:64:LYS:HA    | 1.65                     | 0.77              |
| 49:X:69:LYS:HD2  | 53:3:1320:C:H5'   | 1.66                     | 0.77              |
| 53:3:1091:U:H2'  | 53:3:1092:A:C8    | 2.20                     | 0.77              |
| 28:C:5:ARG:NH1   | 28:C:25:ASN:HB2   | 2.00                     | 0.77              |
| 32:G:128:LEU:HB2 | 32:G:132:GLU:HG2  | 1.66                     | 0.77              |
| 38:M:12:ARG:HD2  | 38:M:26:MET:HG2   | 1.64                     | 0.77              |
| 54:1:1078:U:H4'  | 54:1:1079:C:H5''  | 1.66                     | 0.77              |
| 34:I:56:GLU:OE2  | 34:I:199:ILE:HG13 | 1.85                     | 0.77              |
| 40:O:50:THR:HG21 | 53:3:1367:C:H4'   | 1.65                     | 0.77              |
| 33:H:178:ARG:HB3 | 33:H:178:ARG:NH1  | 1.99                     | 0.77              |
| 54:1:210:C:H2'   | 54:1:211:C:C6     | 2.20                     | 0.77              |
| 59:8:11:ARG:NE   | 59:8:283:ILE:HA   | 1.99                     | 0.77              |
| 4:e:115:GLY:HA3  | 4:e:177:ARG:HB2   | 1.64                     | 0.76              |
| 53:3:1086:U:H2'  | 53:3:1087:G:C8    | 2.19                     | 0.76              |
| 36:K:5:GLU:HA    | 36:K:63:ASN:HA    | 1.66                     | 0.76              |
| 54:1:2682:A:H61  | 54:1:2728:U:H1'   | 1.49                     | 0.76              |
| 3:d:30:GLN:HE22  | 54:1:659:G:N2     | 1.82                     | 0.76              |
| 5:f:49:LEU:HD13  | 5:f:71:LEU:HD21   | 1.67                     | 0.76              |
| 16:q:111:LYS:HE2 | 17:r:48:LYS:HZ1   | 1.50                     | 0.76              |
| 59:8:236:LYS:HG3 | 59:8:243:LEU:HD21 | 1.67                     | 0.76              |
| 23:x:67:LEU:HG   | 23:x:70:LEU:HD12  | 1.65                     | 0.76              |
| 53:3:769:G:H4'   | 53:3:1513:A:H4'   | 1.66                     | 0.76              |
| 3:d:52:VAL:HG21  | 3:d:82:GLY:H      | 1.51                     | 0.76              |
| 6:g:8:LYS:HD2    | 6:g:14:SER:HA     | 1.68                     | 0.76              |
| 53:3:1053:G:HO2' | 53:3:1199:U:H5    | 1.33                     | 0.76              |
| 53:3:1334:G:H2'  | 53:3:1335:U:H5'   | 1.68                     | 0.76              |
| 54:1:2048:G:C2'  | 54:1:2049:G:H5''  | 2.15                     | 0.76              |
| 4:e:110:ILE:HB   | 4:e:113:PHE:HB2   | 1.68                     | 0.76              |
| 37:L:73:GLU:HG2  | 37:L:74:VAL:H     | 1.49                     | 0.75              |
| 40:O:57:VAL:O    | 40:O:58:ASN:HB2   | 1.86                     | 0.75              |
| 41:P:112:VAL:HA  | 48:W:72:ARG:HH12  | 1.49                     | 0.75              |
| 43:R:64:VAL:HG12 | 43:R:65:GLU:H     | 1.51                     | 0.75              |
| 46:U:51:ARG:C    | 46:U:52:LEU:HD12  | 2.11                     | 0.75              |
| 27:B:39:ARG:HG3  | 27:B:40:HIS:ND1   | 2.01                     | 0.75              |
| 51:Z:9:GLU:HB3   | 51:Z:10:PRO:CD    | 2.16                     | 0.75              |
| 52:a:21:TYR:CE1  | 52:a:29:LEU:HD22  | 2.20                     | 0.75              |
| 56:5:2:G:H1'     | 56:5:3:G:OP1      | 1.85                     | 0.75              |
| 53:3:1374:A:H2'  | 53:3:1375:A:C8    | 2.21                     | 0.75              |
| 5:f:163:TYR:HB2  | 5:f:166:GLU:HG3   | 1.66                     | 0.75              |
| 53:3:951:G:O2'   | 53:3:952:U:H5'    | 1.87                     | 0.75              |
| 14:o:31:THR:HG22 | 14:o:33:ARG:H     | 1.50                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:k:76:VAL:HG12  | 15:p:72:VAL:HG22  | 1.68                     | 0.75              |
| 14:o:31:THR:HG23  | 14:o:32:PRO:HD2   | 1.69                     | 0.75              |
| 33:H:87:ARG:HB3   | 33:H:87:ARG:NH1   | 2.01                     | 0.75              |
| 53:3:1374:A:H2'   | 53:3:1375:A:H8    | 1.51                     | 0.75              |
| 22:w:42:HIS:CD2   | 22:w:73:ARG:HD3   | 2.22                     | 0.75              |
| 54:1:1060:U:H4'   | 54:1:1061:U:H5'   | 1.67                     | 0.75              |
| 54:1:2155:U:H2'   | 54:1:2156:G:H5'   | 1.69                     | 0.75              |
| 54:1:2286:G:H5''  | 54:1:2287:A:OP1   | 1.86                     | 0.75              |
| 58:4:17:U:H2'     | 58:4:18:G:H8      | 1.50                     | 0.75              |
| 34:I:152:SER:HB2  | 53:3:436:C:H4'    | 1.69                     | 0.74              |
| 39:N:89:TYR:HB3   | 39:N:93:LEU:HD12  | 1.69                     | 0.74              |
| 52:a:217:THR:HG23 | 54:1:2124:G:H21   | 1.52                     | 0.74              |
| 54:1:1597:A:H5''  | 54:1:1598:A:H5'   | 1.69                     | 0.74              |
| 34:I:18:LEU:HD21  | 34:I:59:LYS:HG3   | 1.67                     | 0.74              |
| 43:R:97:ARG:HA    | 53:3:1308:U:O4'   | 1.86                     | 0.74              |
| 52:a:217:THR:HG22 | 52:a:218:MET:HG3  | 1.68                     | 0.74              |
| 55:2:13:G:H21     | 55:2:16:G:H1'     | 1.51                     | 0.74              |
| 21:v:20:LEU:HD12  | 21:v:21:ARG:N     | 2.02                     | 0.74              |
| 53:3:1164:G:H1'   | 53:3:1165:U:OP1   | 1.86                     | 0.74              |
| 54:1:2167:U:H3    | 54:1:2170:A:H62   | 1.32                     | 0.74              |
| 2:c:4:LEU:HD11    | 2:c:100:LEU:HD22  | 1.69                     | 0.74              |
| 14:o:36:TYR:HD1   | 14:o:52:SER:HB3   | 1.52                     | 0.74              |
| 53:3:919:A:C2     | 53:3:1080:A:N6    | 2.55                     | 0.74              |
| 53:3:934:C:H5     | 53:3:1344:C:H2'   | 1.52                     | 0.74              |
| 53:3:1091:U:H3'   | 53:3:1092:A:C5'   | 2.16                     | 0.74              |
| 53:3:1516:G:H2'   | 53:3:1518:A:OP2   | 1.87                     | 0.74              |
| 55:2:118:C:H2'    | 55:2:119:A:C8     | 2.20                     | 0.74              |
| 54:1:1664:A:H61   | 54:1:1996:C:H42   | 1.36                     | 0.74              |
| 2:c:3:GLY:C       | 2:c:4:LEU:HD12    | 2.12                     | 0.74              |
| 38:M:9:MET:HA     | 38:M:26:MET:HE1   | 1.68                     | 0.74              |
| 46:U:5:ARG:NH1    | 46:U:22:ALA:HB3   | 2.03                     | 0.74              |
| 1:b:270:ARG:HB3   | 1:b:270:ARG:NH1   | 2.02                     | 0.74              |
| 12:m:45:GLN:HE21  | 54:1:2485:G:H5''  | 1.53                     | 0.74              |
| 35:J:113:VAL:HG13 | 35:J:114:LEU:HD22 | 1.70                     | 0.74              |
| 55:2:119:A:C2     | 55:2:120:A:C4     | 2.76                     | 0.74              |
| 56:5:3:G:H4'      | 56:5:4:C:OP1      | 1.86                     | 0.74              |
| 4:e:147:ARG:HH11  | 4:e:148:VAL:H     | 1.36                     | 0.74              |
| 54:1:2493:U:H3'   | 54:1:2494:G:H5''  | 1.69                     | 0.74              |
| 32:G:71:THR:HG23  | 32:G:93:HIS:HA    | 1.68                     | 0.73              |
| 59:8:590:GLU:HG3  | 59:8:591:LEU:HD22 | 1.70                     | 0.73              |
| 33:H:70:ALA:HA    | 33:H:105:VAL:HG12 | 1.70                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 51:Z:32:ARG:HD2  | 51:Z:33:ARG:N    | 2.01                     | 0.73              |
| 16:q:80:ASN:ND2  | 54:1:1151:A:H4'  | 2.04                     | 0.73              |
| 41:P:92:ARG:HE   | 51:Z:24:LYS:NZ   | 1.85                     | 0.73              |
| 43:R:97:ARG:C    | 53:3:1307:U:H3'  | 2.13                     | 0.73              |
| 51:Z:48:LYS:HD2  | 53:3:723:U:O5'   | 1.89                     | 0.73              |
| 53:3:869:G:H4'   | 53:3:872:A:C8    | 2.24                     | 0.73              |
| 18:s:90:LYS:HB2  | 18:s:92:ARG:NH1  | 2.03                     | 0.73              |
| 36:K:9:MET:SD    | 36:K:86:ARG:HB3  | 2.27                     | 0.73              |
| 23:x:35:HIS:CD2  | 23:x:36:ARG:H    | 2.06                     | 0.73              |
| 23:x:16:ASN:ND2  | 23:x:26:ARG:HB3  | 2.02                     | 0.73              |
| 39:N:113:LYS:HG3 | 53:3:1368:A:OP2  | 1.88                     | 0.73              |
| 40:O:7:ARG:HG3   | 40:O:75:ASP:HB2  | 1.71                     | 0.73              |
| 46:U:1:MET:HE2   | 46:U:2:VAL:HG22  | 1.70                     | 0.73              |
| 53:3:1115:U:H2'  | 53:3:1116:U:C5'  | 2.16                     | 0.73              |
| 34:I:74:TYR:HD1  | 34:I:92:LEU:HD23 | 1.53                     | 0.73              |
| 54:1:1434:A:H2'  | 54:1:1435:G:C8   | 2.24                     | 0.73              |
| 6:g:45:GLU:HA    | 6:g:48:GLU:HG2   | 1.69                     | 0.73              |
| 53:3:21:G:H2'    | 53:3:22:G:C8     | 2.23                     | 0.73              |
| 59:8:271:LYS:HA  | 59:8:271:LYS:HE2 | 1.71                     | 0.73              |
| 24:y:1:MET:HA    | 24:y:4:LYS:HB3   | 1.71                     | 0.73              |
| 38:M:17:GLN:NE2  | 38:M:71:VAL:HB   | 2.03                     | 0.73              |
| 54:1:947:A:H2'   | 54:1:948:C:C6    | 2.24                     | 0.73              |
| 8:i:9:LYS:CB     | 54:1:1061:U:H5'' | 2.19                     | 0.72              |
| 18:s:66:ILE:HA   | 18:s:69:LEU:HD13 | 1.71                     | 0.72              |
| 41:P:86:LYS:HG2  | 41:P:112:VAL:O   | 1.89                     | 0.72              |
| 46:U:5:ARG:HB2   | 53:3:376:G:OP1   | 1.89                     | 0.72              |
| 53:3:1315:U:H2'  | 53:3:1316:G:O4'  | 1.89                     | 0.72              |
| 57:6:17:C:H5'    | 57:6:61:C:OP1    | 1.89                     | 0.72              |
| 10:k:76:VAL:HG12 | 15:p:72:VAL:CG2  | 2.18                     | 0.72              |
| 53:3:1065:U:H5'' | 53:3:1190:G:N2   | 2.04                     | 0.72              |
| 55:2:3:C:C2'     | 55:2:4:C:H5''    | 2.19                     | 0.72              |
| 19:t:1:MET:HG3   | 19:t:3:ARG:H     | 1.54                     | 0.72              |
| 26:A:18:CYS:SG   | 26:A:40:CYS:HB2  | 2.29                     | 0.72              |
| 59:8:18:HIS:CE1  | 59:8:19:ILE:HG23 | 2.24                     | 0.72              |
| 44:S:57:SER:HB3  | 53:3:1360:A:C4   | 2.24                     | 0.72              |
| 46:U:1:MET:HE3   | 46:U:2:VAL:H     | 1.55                     | 0.72              |
| 53:3:714:G:H2'   | 53:3:715:A:C8    | 2.24                     | 0.72              |
| 53:3:1392:G:H2'  | 53:3:1393:U:C6   | 2.24                     | 0.72              |
| 54:1:858:G:H5'   | 54:1:859:G:OP2   | 1.89                     | 0.72              |
| 54:1:1300:G:H4'  | 54:1:1301:A:C5'  | 2.17                     | 0.72              |
| 14:o:87:ILE:H    | 14:o:87:ILE:HD12 | 1.54                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:3:964:A:H5''  | 53:3:1199:U:OP1  | 1.89                     | 0.72              |
| 54:1:1872:A:H2'  | 54:1:1873:G:O4'  | 1.89                     | 0.72              |
| 54:1:2743:U:H2'  | 54:1:2744:G:H5'' | 1.71                     | 0.72              |
| 14:o:17:LYS:HZ1  | 54:1:2380:C:H5'  | 1.54                     | 0.72              |
| 41:P:93:GLU:HG2  | 41:P:97:ARG:HH22 | 1.54                     | 0.72              |
| 21:v:63:ILE:HG23 | 21:v:70:ILE:HB   | 1.70                     | 0.72              |
| 52:a:46:VAL:HG13 | 52:a:212:VAL:HA  | 1.70                     | 0.72              |
| 54:1:704:G:H1'   | 54:1:727:A:H61   | 1.54                     | 0.72              |
| 53:3:15:G:H22    | 53:3:1080:A:C1'  | 2.02                     | 0.72              |
| 55:2:118:C:C2    | 55:2:119:A:N7    | 2.58                     | 0.72              |
| 59:8:617:MET:HG3 | 59:8:683:GLU:C   | 2.14                     | 0.72              |
| 13:n:54:LEU:HD11 | 13:n:65:LEU:HD23 | 1.72                     | 0.72              |
| 43:R:88:LEU:HD23 | 43:R:91:ARG:HH21 | 1.54                     | 0.72              |
| 47:V:3:LYS:HG2   | 47:V:4:ILE:H     | 1.53                     | 0.72              |
| 59:8:6:PRO:HB2   | 59:8:9:ARG:HE    | 1.55                     | 0.72              |
| 5:f:136:ASP:OD2  | 5:f:139:VAL:HG23 | 1.89                     | 0.71              |
| 43:R:13:HIS:HB2  | 43:R:16:ILE:HD12 | 1.72                     | 0.71              |
| 53:3:1314:C:H2'  | 53:3:1315:U:O4'  | 1.90                     | 0.71              |
| 14:o:56:LYS:O    | 14:o:60:GLU:HG3  | 1.89                     | 0.71              |
| 38:M:12:ARG:HD2  | 38:M:26:MET:CG   | 2.21                     | 0.71              |
| 53:3:715:A:H2'   | 53:3:716:A:H8    | 1.54                     | 0.71              |
| 53:3:1306:A:H61  | 53:3:1331:G:C1'  | 2.01                     | 0.71              |
| 54:1:690:G:H2'   | 54:1:691:C:H6    | 1.54                     | 0.71              |
| 42:Q:23:LEU:HD12 | 42:Q:29:LYS:HZ3  | 1.56                     | 0.71              |
| 20:u:33:VAL:HG13 | 20:u:66:VAL:HG22 | 1.73                     | 0.71              |
| 46:U:15:PRO:HG2  | 46:U:41:PRO:HG3  | 1.71                     | 0.71              |
| 46:U:22:ALA:HA   | 46:U:33:ILE:CD1  | 2.19                     | 0.71              |
| 54:1:974:G:H8    | 54:1:990:A:H62   | 1.37                     | 0.71              |
| 55:2:65:U:H3'    | 55:2:108:A:H61   | 1.55                     | 0.71              |
| 59:8:691:PRO:HG2 | 59:8:694:VAL:HB  | 1.71                     | 0.71              |
| 40:O:44:THR:HG22 | 40:O:70:HIS:HA   | 1.72                     | 0.71              |
| 44:S:53:ASP:HA   | 44:S:58:ARG:HD3  | 1.73                     | 0.71              |
| 53:3:868:C:H2'   | 53:3:869:G:O4'   | 1.90                     | 0.71              |
| 53:3:1114:C:O2   | 53:3:1115:U:N3   | 2.24                     | 0.71              |
| 14:o:43:ASN:HD21 | 14:o:45:SER:HB3  | 1.54                     | 0.71              |
| 40:O:66:GLU:HG2  | 44:S:98:ALA:HB2  | 1.73                     | 0.71              |
| 53:3:501:C:H2'   | 53:3:502:A:H8    | 1.54                     | 0.71              |
| 46:U:5:ARG:HG3   | 53:3:376:G:H5''  | 1.73                     | 0.71              |
| 54:1:1028:A:H2'  | 54:1:1029:A:C8   | 2.26                     | 0.71              |
| 54:1:2118:U:H5   | 54:1:2149:U:H1'  | 1.56                     | 0.71              |
| 21:v:26:PHE:CZ   | 21:v:42:LEU:HD11 | 2.26                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 43:R:98:GLY:HA3  | 53:3:1307:U:P     | 2.30                     | 0.71              |
| 48:W:33:THR:CG2  | 48:W:37:LYS:H     | 2.04                     | 0.71              |
| 53:3:1412:C:H2'  | 53:3:1413:A:C8    | 2.25                     | 0.71              |
| 54:1:1213:A:N6   | 54:1:1236:G:H1'   | 2.05                     | 0.71              |
| 22:w:39:THR:H    | 54:1:2331:G:H4'   | 1.54                     | 0.71              |
| 30:E:30:HIS:ND1  | 30:E:31:ILE:HG12  | 2.06                     | 0.71              |
| 45:T:7:THR:O     | 45:T:11:VAL:HG23  | 1.90                     | 0.71              |
| 53:3:1136:C:H5'' | 53:3:1137:C:OP2   | 1.91                     | 0.71              |
| 10:k:104:THR:CG2 | 10:k:106:GLU:H    | 2.04                     | 0.71              |
| 20:u:4:ILE:HD12  | 20:u:4:ILE:H      | 1.56                     | 0.71              |
| 54:1:1434:A:H2'  | 54:1:1435:G:H8    | 1.54                     | 0.71              |
| 54:1:1807:G:H2'  | 54:1:1808:A:H5'   | 1.72                     | 0.71              |
| 54:1:2328:A:H2'  | 54:1:2329:U:C6    | 2.26                     | 0.71              |
| 5:f:24:THR:HG23  | 5:f:33:THR:HG22   | 1.73                     | 0.70              |
| 44:S:100:TRP:HA  | 53:3:1115:U:O2    | 1.91                     | 0.70              |
| 53:3:273:U:H2'   | 53:3:274:A:H5'    | 1.72                     | 0.70              |
| 54:1:580:U:H2'   | 54:1:581:C:C6     | 2.26                     | 0.70              |
| 9:j:27:ARG:HH22  | 54:1:1142:A:H4'   | 1.56                     | 0.70              |
| 33:H:42:LEU:HD23 | 33:H:54:ILE:HD12  | 1.71                     | 0.70              |
| 43:R:76:ILE:O    | 43:R:79:LEU:HG    | 1.91                     | 0.70              |
| 4:e:116:LEU:HB3  | 4:e:176:PHE:H     | 1.56                     | 0.70              |
| 9:j:45:THR:HB    | 9:j:48:VAL:HG22   | 1.74                     | 0.70              |
| 13:n:37:THR:OG1  | 13:n:39:PRO:HD2   | 1.90                     | 0.70              |
| 32:G:108:GLN:HG3 | 32:G:112:ARG:NH1  | 2.06                     | 0.70              |
| 44:S:5:MET:HG2   | 44:S:62:ARG:HH22  | 1.57                     | 0.70              |
| 44:S:48:GLN:HG3  | 53:3:1317:C:O2'   | 1.90                     | 0.70              |
| 52:a:165:ASN:HB3 | 52:a:171:ILE:HG22 | 1.73                     | 0.70              |
| 53:3:225:C:H2'   | 53:3:226:G:H5''   | 1.72                     | 0.70              |
| 54:1:481:G:H1'   | 54:1:506:G:N2     | 2.05                     | 0.70              |
| 54:1:2104:C:H2'  | 54:1:2105:U:C6    | 2.27                     | 0.70              |
| 54:1:2564:A:C2   | 54:1:2647:U:H4'   | 2.26                     | 0.70              |
| 59:8:446:ARG:HB2 | 59:8:459:ALA:HB3  | 1.73                     | 0.70              |
| 35:J:14:LEU:HA   | 35:J:36:THR:HG22  | 1.73                     | 0.70              |
| 53:3:399:G:H2'   | 53:3:400:C:C6     | 2.25                     | 0.70              |
| 53:3:673:A:H2'   | 53:3:674:G:C8     | 2.25                     | 0.70              |
| 54:1:703:U:H2'   | 54:1:704:G:O4'    | 1.91                     | 0.70              |
| 54:1:2277:G:H2'  | 54:1:2278:A:H5''  | 1.73                     | 0.70              |
| 37:L:65:LEU:O    | 37:L:65:LEU:HD23  | 1.91                     | 0.70              |
| 52:a:48:LEU:HD22 | 52:a:209:ILE:HG12 | 1.74                     | 0.70              |
| 53:3:1071:C:H2'  | 53:3:1072:G:H8    | 1.55                     | 0.70              |
| 53:3:1512:U:H2'  | 53:3:1513:A:H8    | 1.56                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:f:92:GLY:HA2    | 5:f:94:ARG:NH1    | 2.07                     | 0.70              |
| 7:h:81:LEU:H      | 7:h:81:LEU:HD12   | 1.57                     | 0.70              |
| 42:Q:32:VAL:HB    | 42:Q:55:ARG:HB3   | 1.74                     | 0.70              |
| 43:R:97:ARG:O     | 53:3:1307:U:C6    | 2.45                     | 0.70              |
| 52:a:49:GLY:HA2   | 52:a:210:LYS:NZ   | 2.06                     | 0.70              |
| 54:1:279:A:H2'    | 54:1:280:U:O4'    | 1.91                     | 0.70              |
| 1:b:48:ILE:HG13   | 54:1:779:U:OP1    | 1.92                     | 0.70              |
| 43:R:82:LEU:HD11  | 49:X:65:MET:HB3   | 1.74                     | 0.70              |
| 54:1:1773:A:H2'   | 54:1:1774:C:H5'   | 1.74                     | 0.70              |
| 1:b:225:ASN:HB2   | 1:b:228:ASP:OD2   | 1.91                     | 0.70              |
| 33:H:19:SER:O     | 44:S:93:PRO:HG3   | 1.92                     | 0.70              |
| 35:J:45:VAL:HG23  | 35:J:71:ILE:HB    | 1.73                     | 0.70              |
| 8:i:48:ILE:HG13   | 8:i:49:GLU:H      | 1.56                     | 0.70              |
| 10:k:88:ASN:HD22  | 10:k:89:ASN:N     | 1.89                     | 0.70              |
| 46:U:4:ILE:HG12   | 46:U:21:VAL:HG22  | 1.74                     | 0.70              |
| 52:a:60:ARG:HE    | 52:a:164:ARG:NH1  | 1.90                     | 0.70              |
| 53:3:1462:C:H2'   | 53:3:1463:U:C6    | 2.27                     | 0.70              |
| 54:1:1775:U:H2'   | 54:1:1776:G:H5'   | 1.73                     | 0.70              |
| 59:8:158:ILE:HD12 | 59:8:162:LEU:HD12 | 1.74                     | 0.70              |
| 8:i:16:MET:HE3    | 8:i:17:ALA:H      | 1.57                     | 0.70              |
| 49:X:35:ARG:HE    | 49:X:71:GLY:HA2   | 1.57                     | 0.70              |
| 53:3:102:G:H2'    | 53:3:103:U:C6     | 2.27                     | 0.70              |
| 53:3:962:C:H1'    | 53:3:1201:A:C6    | 2.27                     | 0.70              |
| 53:3:1170:A:H2'   | 53:3:1171:A:O4'   | 1.92                     | 0.70              |
| 53:3:1227:A:H2'   | 53:3:1228:C:H5'   | 1.74                     | 0.70              |
| 55:2:23:G:H2'     | 55:2:24:G:C8      | 2.27                     | 0.70              |
| 3:d:105:LEU:O     | 3:d:109:LEU:HD13  | 1.91                     | 0.69              |
| 6:g:5:LEU:HD13    | 6:g:13:GLY:HA2    | 1.73                     | 0.69              |
| 43:R:24:VAL:HG12  | 43:R:28:ARG:HD3   | 1.73                     | 0.69              |
| 44:S:82:LYS:O     | 44:S:85:GLU:HG3   | 1.92                     | 0.69              |
| 59:8:497:LYS:HG2  | 59:8:524:PRO:HD2  | 1.72                     | 0.69              |
| 3:d:149:ILE:HD11  | 3:d:172:ALA:HA    | 1.73                     | 0.69              |
| 21:v:30:ILE:HD12  | 21:v:38:LEU:HD23  | 1.73                     | 0.69              |
| 31:F:36:ARG:HD2   | 31:F:37:GLN:H     | 1.56                     | 0.69              |
| 50:Y:26:MET:HE1   | 50:Y:56:ILE:HG23  | 1.74                     | 0.69              |
| 54:1:2286:G:H4'   | 54:1:2287:A:O4'   | 1.91                     | 0.69              |
| 55:2:66:A:H5''    | 55:2:67:G:OP1     | 1.92                     | 0.69              |
| 5:f:46:ASP:CG     | 5:f:47:ASN:H      | 2.00                     | 0.69              |
| 15:p:62:LYS:HE2   | 15:p:64:SER:HB3   | 1.73                     | 0.69              |
| 39:N:50:PRO:HD3   | 39:N:79:ARG:HG3   | 1.73                     | 0.69              |
| 59:8:318:SER:HB3  | 59:8:340:SER:HB3  | 1.73                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 59:8:621:VAL:HG12 | 59:8:680:TYR:HB3  | 1.73                     | 0.69              |
| 40:O:36:VAL:HG13  | 53:3:1123:U:H5'   | 1.73                     | 0.69              |
| 53:3:219:U:H2'    | 53:3:220:G:H8     | 1.56                     | 0.69              |
| 53:3:1176:A:H2'   | 53:3:1177:G:C8    | 2.27                     | 0.69              |
| 1:b:121:ALA:HB3   | 1:b:129:LEU:HD23  | 1.73                     | 0.69              |
| 1:b:160:TYR:HB3   | 1:b:193:GLU:HG3   | 1.74                     | 0.69              |
| 2:c:39:ASP:OD2    | 2:c:41:ALA:HB3    | 1.92                     | 0.69              |
| 34:I:104:MET:HE2  | 34:I:179:GLY:HA2  | 1.73                     | 0.69              |
| 36:K:9:MET:HB2    | 36:K:85:ILE:HG13  | 1.75                     | 0.69              |
| 53:3:57:G:H2'     | 53:3:58:C:H6      | 1.56                     | 0.69              |
| 53:3:1065:U:H5''  | 53:3:1190:G:C2    | 2.27                     | 0.69              |
| 4:e:66:ILE:HG22   | 4:e:86:CYS:SG     | 2.31                     | 0.69              |
| 15:p:96:LEU:HB3   | 15:p:99:LEU:HD23  | 1.72                     | 0.69              |
| 47:V:31:PRO:HB2   | 47:V:32:ILE:HD12  | 1.74                     | 0.69              |
| 54:1:1075:C:C3'   | 54:1:1076:C:H5''  | 2.22                     | 0.69              |
| 54:1:2493:U:C3'   | 54:1:2494:G:H5''  | 2.23                     | 0.69              |
| 59:8:492:GLU:OE1  | 59:8:566:LEU:HB3  | 1.91                     | 0.69              |
| 8:i:25:PRO:HG3    | 59:8:647:SER:HB3  | 1.74                     | 0.69              |
| 47:V:59:GLU:HG3   | 47:V:76:ARG:NH1   | 2.07                     | 0.69              |
| 50:Y:38:ILE:HD13  | 50:Y:81:GLN:HB3   | 1.74                     | 0.69              |
| 59:8:235:GLU:HA   | 59:8:238:LEU:HB2  | 1.74                     | 0.69              |
| 5:f:89:VAL:HG21   | 5:f:162:ARG:HH11  | 1.57                     | 0.69              |
| 9:j:26:GLY:HA3    | 54:1:1140:C:H5'   | 1.75                     | 0.69              |
| 14:o:74:VAL:O     | 14:o:78:VAL:HG23  | 1.93                     | 0.69              |
| 34:I:50:TYR:HD2   | 53:3:509:A:H5'    | 1.57                     | 0.69              |
| 34:I:195:ASN:HD22 | 34:I:198:LEU:HG   | 1.58                     | 0.69              |
| 44:S:29:ILE:HA    | 44:S:32:ASP:OD2   | 1.92                     | 0.69              |
| 52:a:11:ILE:HG21  | 52:a:218:MET:O    | 1.92                     | 0.69              |
| 52:a:217:THR:HG23 | 54:1:2124:G:N2    | 2.06                     | 0.69              |
| 53:3:1206:G:C2    | 53:3:1207:G:H1'   | 2.28                     | 0.69              |
| 53:3:1251:A:O2'   | 53:3:1370:G:H5'   | 1.93                     | 0.69              |
| 53:3:1435:G:H2'   | 53:3:1436:U:C6    | 2.27                     | 0.69              |
| 54:1:1801:A:H5''  | 54:1:2203:U:H2'   | 1.75                     | 0.69              |
| 54:1:2529:G:OP2   | 54:1:2530:A:H5''  | 1.93                     | 0.69              |
| 17:r:58:VAL:H     | 17:r:102:SER:HB2  | 1.58                     | 0.69              |
| 29:D:3:ARG:HA     | 29:D:3:ARG:NE     | 2.07                     | 0.69              |
| 37:L:45:ALA:HB1   | 37:L:123:LEU:HD11 | 1.75                     | 0.69              |
| 53:3:15:G:H1      | 53:3:1080:A:H1'   | 1.58                     | 0.69              |
| 53:3:102:G:H2'    | 53:3:103:U:H6     | 1.58                     | 0.69              |
| 54:1:191:A:H2'    | 54:1:192:C:C6     | 2.28                     | 0.69              |
| 54:1:2386:A:H2'   | 54:1:2387:U:C6    | 2.27                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 54:1:2243:U:H2'  | 54:1:2244:U:C6   | 2.28                     | 0.69              |
| 54:1:2467:C:H2'  | 54:1:2468:A:O4'  | 1.93                     | 0.69              |
| 59:8:193:TRP:HB2 | 59:8:273:LYS:HE3 | 1.74                     | 0.69              |
| 32:G:89:PHE:CD2  | 32:G:153:MET:HE3 | 2.28                     | 0.68              |
| 32:G:105:THR:O   | 32:G:108:GLN:HG2 | 1.93                     | 0.68              |
| 59:8:17:ALA:HB2  | 59:8:112:VAL:H   | 1.58                     | 0.68              |
| 4:e:28:PRO:HB2   | 4:e:168:LEU:HD22 | 1.75                     | 0.68              |
| 41:P:51:PHE:HB3  | 41:P:55:ARG:HB2  | 1.75                     | 0.68              |
| 42:Q:29:LYS:HE2  | 42:Q:58:ASN:ND2  | 2.08                     | 0.68              |
| 46:U:76:LYS:HD2  | 46:U:80:LYS:NZ   | 2.07                     | 0.68              |
| 4:e:39:VAL:HG13  | 4:e:40:GLY:H     | 1.59                     | 0.68              |
| 33:H:71:ARG:HB3  | 33:H:74:ILE:HD13 | 1.76                     | 0.68              |
| 35:J:81:GLN:HB2  | 35:J:146:MET:SD  | 2.34                     | 0.68              |
| 40:O:7:ARG:HB3   | 40:O:101:SER:HB3 | 1.73                     | 0.68              |
| 46:U:61:VAL:HG22 | 46:U:67:ILE:HD11 | 1.74                     | 0.68              |
| 53:3:1164:G:C2   | 53:3:1165:U:O4   | 2.46                     | 0.68              |
| 53:3:1218:C:H2'  | 53:3:1219:A:H8   | 1.54                     | 0.68              |
| 54:1:1893:C:H2'  | 54:1:1894:C:H5'  | 1.73                     | 0.68              |
| 53:3:252:U:O2    | 53:3:252:U:H2'   | 1.94                     | 0.68              |
| 53:3:1071:C:H2'  | 53:3:1072:G:C8   | 2.27                     | 0.68              |
| 57:6:27:U:H2'    | 57:6:28:C:H5''   | 1.73                     | 0.68              |
| 9:j:1:MET:HE3    | 9:j:2:LYS:H      | 1.57                     | 0.68              |
| 32:G:131:LYS:HD3 | 32:G:131:LYS:H   | 1.58                     | 0.68              |
| 44:S:15:LEU:HD13 | 44:S:53:ASP:HB2  | 1.75                     | 0.68              |
| 53:3:501:C:H2'   | 53:3:502:A:C8    | 2.28                     | 0.68              |
| 53:3:955:U:H3    | 53:3:1225:A:H61  | 1.40                     | 0.68              |
| 53:3:1125:U:O4   | 53:3:1280:A:N7   | 2.26                     | 0.68              |
| 54:1:1786:A:H1'  | 54:1:1938:A:N6   | 2.07                     | 0.68              |
| 33:H:50:SER:HB2  | 33:H:71:ARG:HE   | 1.57                     | 0.68              |
| 53:3:1169:A:H2'  | 53:3:1170:A:O4'  | 1.94                     | 0.68              |
| 53:3:1517:G:H2'  | 53:3:1518:A:H5'  | 1.75                     | 0.68              |
| 59:8:19:ILE:HA   | 62:8:801:GCP:O2G | 1.94                     | 0.68              |
| 1:b:123:ILE:HG23 | 1:b:191:LEU:HD11 | 1.75                     | 0.68              |
| 43:R:92:ARG:HB3  | 43:R:94:LEU:HG   | 1.76                     | 0.68              |
| 48:W:20:ILE:HG22 | 48:W:21:ASP:H    | 1.59                     | 0.68              |
| 53:3:744:C:H2'   | 53:3:745:G:C8    | 2.28                     | 0.68              |
| 54:1:121:G:H4'   | 54:1:149:A:H5'   | 1.75                     | 0.68              |
| 54:1:1919:A:H2'  | 54:1:1920:C:H5'  | 1.74                     | 0.68              |
| 13:n:65:LEU:HG   | 13:n:69:ARG:HH22 | 1.59                     | 0.68              |
| 28:C:4:ILE:H     | 28:C:4:ILE:HD12  | 1.58                     | 0.68              |
| 35:J:76:ASN:HB2  | 35:J:81:GLN:NE2  | 2.09                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:3:152:A:H2'   | 53:3:153:C:H5'   | 1.75                     | 0.68              |
| 53:3:219:U:H2'   | 53:3:220:G:C8    | 2.29                     | 0.68              |
| 54:1:760:G:H2'   | 54:1:761:A:O4'   | 1.93                     | 0.68              |
| 54:1:1071:G:OP1  | 54:1:1071:G:H3'  | 1.92                     | 0.68              |
| 54:1:2287:A:O2'  | 54:1:2288:A:H2'  | 1.93                     | 0.68              |
| 12:m:42:THR:HA   | 12:m:93:VAL:HG12 | 1.76                     | 0.68              |
| 42:Q:87:LYS:HE3  | 53:3:526:C:OP2   | 1.94                     | 0.68              |
| 53:3:1200:C:H5'' | 53:3:1201:A:C3'  | 2.24                     | 0.68              |
| 54:1:1484:U:H2'  | 54:1:1485:U:C6   | 2.29                     | 0.68              |
| 54:1:2224:G:H4'  | 54:1:2226:C:O2   | 1.94                     | 0.68              |
| 31:F:1:MET:HE2   | 31:F:36:ARG:HB2  | 1.75                     | 0.68              |
| 54:1:222:A:H61   | 54:1:232:G:H1'   | 1.59                     | 0.68              |
| 54:1:1300:G:H4'  | 54:1:1301:A:H5'' | 1.76                     | 0.68              |
| 2:c:24:VAL:HG12  | 2:c:178:VAL:HG21 | 1.75                     | 0.67              |
| 53:3:976:G:N2    | 53:3:1362:A:H2'  | 2.08                     | 0.67              |
| 47:V:29:LYS:HA   | 47:V:36:PHE:HA   | 1.76                     | 0.67              |
| 54:1:1532:A:H2   | 54:1:1539:U:H3   | 1.40                     | 0.67              |
| 55:2:114:C:H2'   | 55:2:115:A:C8    | 2.29                     | 0.67              |
| 7:h:34:THR:HG22  | 54:1:1085:A:H61  | 1.59                     | 0.67              |
| 32:G:219:THR:O   | 32:G:223:GLY:N   | 2.27                     | 0.67              |
| 47:V:16:MET:HE1  | 53:3:253:A:N3    | 2.09                     | 0.67              |
| 54:1:690:G:H2'   | 54:1:691:C:C6    | 2.29                     | 0.67              |
| 59:8:308:GLU:HB2 | 59:8:310:HIS:CE1 | 2.29                     | 0.67              |
| 3:d:188:MET:HE3  | 3:d:193:VAL:HG22 | 1.77                     | 0.67              |
| 40:O:80:THR:HG22 | 40:O:82:LYS:H    | 1.59                     | 0.67              |
| 22:w:17:LEU:H    | 22:w:17:LEU:HD12 | 1.59                     | 0.67              |
| 40:O:57:VAL:HG22 | 40:O:58:ASN:N    | 2.09                     | 0.67              |
| 53:3:313:A:H2'   | 53:3:314:C:C6    | 2.29                     | 0.67              |
| 53:3:677:U:H3    | 53:3:713:G:H22   | 1.41                     | 0.67              |
| 53:3:929:G:H2'   | 53:3:930:C:C6    | 2.30                     | 0.67              |
| 54:1:2281:A:O2'  | 54:1:2282:G:H5'  | 1.94                     | 0.67              |
| 16:q:69:ARG:NH2  | 16:q:74:SER:HA   | 2.08                     | 0.67              |
| 41:P:112:VAL:HB  | 48:W:72:ARG:HH22 | 1.57                     | 0.67              |
| 50:Y:80:ALA:HA   | 50:Y:83:ASN:ND2  | 2.10                     | 0.67              |
| 53:3:57:G:H2'    | 53:3:58:C:C6     | 2.30                     | 0.67              |
| 54:1:828:U:H2'   | 54:1:829:A:C8    | 2.29                     | 0.67              |
| 54:1:2106:U:H2'  | 54:1:2107:G:H8   | 1.58                     | 0.67              |
| 54:1:2241:A:H2'  | 54:1:2242:G:C8   | 2.30                     | 0.67              |
| 16:q:29:ARG:HH11 | 16:q:29:ARG:HG3  | 1.60                     | 0.67              |
| 32:G:25:LYS:HE2  | 32:G:25:LYS:HA   | 1.76                     | 0.67              |
| 41:P:78:ILE:HG21 | 41:P:81:LEU:HB3  | 1.77                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 54:1:1614:A:H2'  | 54:1:1615:C:H5'   | 1.74                     | 0.67              |
| 43:R:95:PRO:HG2  | 43:R:101:THR:HG21 | 1.76                     | 0.67              |
| 53:3:931:C:H2'   | 53:3:932:C:C6     | 2.30                     | 0.67              |
| 54:1:1075:C:H3'  | 54:1:1076:C:C5'   | 2.25                     | 0.67              |
| 32:G:27:LYS:HB3  | 32:G:28:PRO:HD3   | 1.77                     | 0.67              |
| 38:M:95:MET:HE3  | 38:M:98:LEU:HD21  | 1.75                     | 0.67              |
| 43:R:94:LEU:HD23 | 43:R:108:ARG:NH2  | 2.10                     | 0.67              |
| 54:1:1837:C:H2'  | 54:1:1899:A:H61   | 1.59                     | 0.67              |
| 3:d:40:ARG:HH12  | 54:1:443:A:H3'    | 1.60                     | 0.67              |
| 3:d:125:SER:H    | 3:d:137:LYS:HZ3   | 1.42                     | 0.67              |
| 11:l:47:ARG:HH21 | 11:l:47:ARG:CB    | 2.08                     | 0.67              |
| 20:u:42:LYS:HE2  | 54:1:499:U:H5''   | 1.75                     | 0.67              |
| 43:R:99:GLN:HG3  | 43:R:100:ARG:H    | 1.58                     | 0.67              |
| 53:3:1149:C:H2'  | 53:3:1150:A:O4'   | 1.95                     | 0.67              |
| 54:1:1796:U:H2'  | 54:1:1797:G:H8    | 1.60                     | 0.67              |
| 54:1:2788:C:H2'  | 54:1:2789:C:C6    | 2.30                     | 0.67              |
| 55:2:119:A:C2    | 55:2:120:A:N3     | 2.62                     | 0.67              |
| 53:3:31:G:H21    | 53:3:47:C:H5''    | 1.61                     | 0.66              |
| 55:2:115:A:H2'   | 55:2:116:G:H8     | 1.60                     | 0.66              |
| 1:b:96:LYS:HB3   | 54:1:1490:A:H62   | 1.61                     | 0.66              |
| 4:e:3:LEU:HD11   | 4:e:99:PHE:HD2    | 1.60                     | 0.66              |
| 10:k:76:VAL:H    | 15:p:72:VAL:HG22  | 1.59                     | 0.66              |
| 11:l:95:LEU:HD22 | 11:l:100:ILE:HD11 | 1.76                     | 0.66              |
| 14:o:55:GLU:HG2  | 55:2:116:G:H5'    | 1.77                     | 0.66              |
| 15:p:38:ARG:HG2  | 15:p:39:LEU:N     | 2.10                     | 0.66              |
| 33:H:149:LYS:HZ3 | 33:H:166:TRP:HE3  | 1.41                     | 0.66              |
| 43:R:95:PRO:HB2  | 53:3:1308:U:OP1   | 1.95                     | 0.66              |
| 53:3:459:A:H2'   | 53:3:460:A:C8     | 2.31                     | 0.66              |
| 59:8:623:THR:OG1 | 59:8:627:ASN:HB2  | 1.95                     | 0.66              |
| 6:g:14:SER:HB3   | 6:g:17:ASP:OD2    | 1.96                     | 0.66              |
| 34:I:36:ALA:HA   | 34:I:41:GLY:HA3   | 1.76                     | 0.66              |
| 51:Z:44:ARG:HD2  | 51:Z:44:ARG:O     | 1.94                     | 0.66              |
| 53:3:1504:G:OP1  | 53:3:1507:A:H4'   | 1.96                     | 0.66              |
| 54:1:215:G:H4'   | 54:1:216:A:H4'    | 1.77                     | 0.66              |
| 1:b:106:PRO:HG2  | 1:b:109:LEU:HB2   | 1.78                     | 0.66              |
| 5:f:41:GLU:HG2   | 5:f:54:ARG:HB2    | 1.77                     | 0.66              |
| 11:l:23:ILE:HG13 | 17:r:82:HIS:CD2   | 2.30                     | 0.66              |
| 29:D:24:THR:HG23 | 29:D:27:GLY:H     | 1.60                     | 0.66              |
| 33:H:113:LYS:HB2 | 33:H:184:ASN:ND2  | 2.11                     | 0.66              |
| 35:J:98:ALA:HB3  | 35:J:122:VAL:HA   | 1.78                     | 0.66              |
| 44:S:58:ARG:NH2  | 53:3:979:C:H2'    | 2.10                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:3:1200:C:H5'' | 53:3:1201:A:H3'   | 1.77                     | 0.66              |
| 54:1:49:A:H5'    | 54:1:51:G:O4'     | 1.96                     | 0.66              |
| 54:1:2134:A:C6   | 54:1:2157:G:H4'   | 2.30                     | 0.66              |
| 59:8:63:ILE:HG21 | 59:8:468:ILE:HG21 | 1.77                     | 0.66              |
| 27:B:12:ARG:HD2  | 27:B:16:ARG:NH2   | 2.11                     | 0.66              |
| 39:N:28:VAL:HA   | 39:N:33:SER:HA    | 1.76                     | 0.66              |
| 41:P:12:ARG:HB2  | 41:P:13:LYS:NZ    | 2.11                     | 0.66              |
| 50:Y:66:ILE:HG22 | 50:Y:68:LYS:H     | 1.59                     | 0.66              |
| 51:Z:34:ARG:HD3  | 51:Z:36:PHE:CZ    | 2.31                     | 0.66              |
| 53:3:555:U:H2'   | 53:3:556:C:C6     | 2.29                     | 0.66              |
| 53:3:928:G:H2'   | 53:3:929:G:C8     | 2.30                     | 0.66              |
| 53:3:1091:U:C3'  | 53:3:1092:A:H5''  | 2.24                     | 0.66              |
| 2:c:118:PHE:CE1  | 2:c:163:GLY:HA2   | 2.30                     | 0.66              |
| 11:l:23:ILE:HG13 | 17:r:82:HIS:NE2   | 2.11                     | 0.66              |
| 36:K:18:VAL:HG13 | 36:K:19:PRO:HD3   | 1.77                     | 0.66              |
| 40:O:15:HIS:HA   | 40:O:18:ILE:HG22  | 1.77                     | 0.66              |
| 40:O:85:ASP:HB2  | 40:O:89:ARG:NH1   | 2.11                     | 0.66              |
| 45:T:46:LYS:HB3  | 45:T:47:LYS:HZ2   | 1.59                     | 0.66              |
| 54:1:1075:C:H3'  | 54:1:1076:C:H5''  | 1.78                     | 0.66              |
| 54:1:2066:C:O2'  | 54:1:2067:G:H5'   | 1.95                     | 0.66              |
| 13:n:31:HIS:CD2  | 54:1:1279:G:H4'   | 2.31                     | 0.66              |
| 14:o:3:LYS:HD2   | 55:2:47:C:P       | 2.35                     | 0.66              |
| 37:L:92:PRO:HA   | 37:L:95:ARG:HB3   | 1.77                     | 0.66              |
| 54:1:2071:A:H2'  | 54:1:2072:C:C6    | 2.30                     | 0.66              |
| 54:1:2106:U:H2'  | 54:1:2107:G:C8    | 2.31                     | 0.66              |
| 59:8:366:MET:HE1 | 59:8:371:ARG:HG3  | 1.76                     | 0.66              |
| 2:c:31:ALA:HB1   | 2:c:95:SER:OG     | 1.96                     | 0.66              |
| 11:l:58:TYR:O    | 30:E:12:ARG:HD2   | 1.96                     | 0.66              |
| 34:I:187:ARG:HD2 | 34:I:190:LEU:HD11 | 1.78                     | 0.66              |
| 39:N:55:ASP:HB3  | 39:N:59:LYS:HG2   | 1.77                     | 0.66              |
| 55:2:114:C:H2'   | 55:2:115:A:H8     | 1.61                     | 0.66              |
| 59:8:175:ALA:O   | 59:8:179:PHE:N    | 2.27                     | 0.66              |
| 59:8:217:GLU:O   | 59:8:220:GLN:HG3  | 1.95                     | 0.66              |
| 25:z:23:LEU:HD21 | 25:z:53:MET:HE2   | 1.77                     | 0.66              |
| 44:S:8:ARG:NE    | 53:3:1217:C:H5''  | 2.07                     | 0.66              |
| 53:3:990:C:H2'   | 53:3:991:U:O4'    | 1.96                     | 0.66              |
| 54:1:1171:G:H2'  | 54:1:1172:C:O4'   | 1.96                     | 0.66              |
| 13:n:83:LEU:HD22 | 13:n:87:PHE:CE2   | 2.23                     | 0.66              |
| 52:a:54:LYS:HE3  | 52:a:205:LYS:HD2  | 1.76                     | 0.66              |
| 54:1:394:C:H2'   | 54:1:395:U:O4'    | 1.96                     | 0.66              |
| 41:P:111:ASP:O   | 51:Z:3:ILE:HG22   | 1.96                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:524:G:H2'    | 53:3:525:C:C6     | 2.30                     | 0.65              |
| 54:1:955:U:H3     | 54:1:962:G:H1     | 1.43                     | 0.65              |
| 55:2:1:U:C5       | 55:2:2:G:N7       | 2.64                     | 0.65              |
| 53:3:337:G:H2'    | 53:3:338:A:C8     | 2.31                     | 0.65              |
| 53:3:1221:G:H2'   | 53:3:1222:G:C8    | 2.31                     | 0.65              |
| 53:3:1280:A:O2'   | 53:3:1281:C:H5'   | 1.96                     | 0.65              |
| 54:1:488:G:H22    | 54:1:491:G:H5''   | 1.62                     | 0.65              |
| 54:1:2243:U:H2'   | 54:1:2244:U:H6    | 1.61                     | 0.65              |
| 11:l:81:ASP:HA    | 11:l:84:LYS:HE2   | 1.78                     | 0.65              |
| 36:K:6:ILE:HG23   | 36:K:62:MET:HE2   | 1.78                     | 0.65              |
| 38:M:6:ILE:HD13   | 38:M:32:LYS:HE3   | 1.79                     | 0.65              |
| 42:Q:98:ARG:NH1   | 42:Q:106:VAL:HG22 | 2.11                     | 0.65              |
| 44:S:3:GLN:NE2    | 44:S:6:LYS:HD2    | 2.11                     | 0.65              |
| 53:3:212:G:H2'    | 53:3:213:G:H8     | 1.62                     | 0.65              |
| 53:3:979:C:O5'    | 53:3:979:C:H6     | 1.78                     | 0.65              |
| 13:n:72:ASP:OD2   | 13:n:75:ILE:HG12  | 1.97                     | 0.65              |
| 19:t:8:LEU:HD13   | 24:y:21:LEU:HB3   | 1.79                     | 0.65              |
| 40:O:73:LEU:O     | 53:3:1123:U:H2'   | 1.97                     | 0.65              |
| 41:P:54:SER:HB3   | 53:3:694:A:H5''   | 1.78                     | 0.65              |
| 53:3:1391:U:H2'   | 53:3:1392:G:C8    | 2.32                     | 0.65              |
| 54:1:2590:A:H61   | 54:1:2604:U:H3    | 1.43                     | 0.65              |
| 8:i:55:PRO:HD3    | 8:i:74:PRO:HD3    | 1.78                     | 0.65              |
| 8:i:57:VAL:HG12   | 8:i:69:VAL:O      | 1.96                     | 0.65              |
| 9:j:17:VAL:HA     | 9:j:55:ILE:CG2    | 2.27                     | 0.65              |
| 53:3:70:U:H5''    | 53:3:71:A:OP1     | 1.96                     | 0.65              |
| 53:3:878:A:H2'    | 53:3:879:C:C6     | 2.31                     | 0.65              |
| 54:1:2537:U:H2'   | 54:1:2538:C:C6    | 2.32                     | 0.65              |
| 1:b:167:ASP:OD1   | 1:b:170:TYR:HB2   | 1.96                     | 0.65              |
| 9:j:101:ILE:H     | 9:j:101:ILE:HD12  | 1.61                     | 0.65              |
| 15:p:30:TRP:CZ3   | 15:p:39:LEU:HB2   | 2.32                     | 0.65              |
| 49:X:77:ARG:HD2   | 53:3:1225:A:O2'   | 1.97                     | 0.65              |
| 51:Z:32:ARG:HD2   | 51:Z:33:ARG:H     | 1.59                     | 0.65              |
| 53:3:1517:G:C2'   | 53:3:1518:A:H5'   | 2.27                     | 0.65              |
| 59:8:660:LEU:HD13 | 59:8:682:MET:HE1  | 1.79                     | 0.65              |
| 24:y:42:LEU:O     | 24:y:46:VAL:HG23  | 1.97                     | 0.65              |
| 35:J:80:LEU:HD13  | 35:J:122:VAL:CG1  | 2.27                     | 0.65              |
| 35:J:164:LEU:HD12 | 35:J:165:GLY:N    | 2.12                     | 0.65              |
| 51:Z:48:LYS:HD3   | 53:3:723:U:C6     | 2.27                     | 0.65              |
| 54:1:1450:G:H21   | 54:1:1452:G:H1    | 1.43                     | 0.65              |
| 3:d:125:SER:H     | 3:d:137:LYS:NZ    | 1.93                     | 0.65              |
| 35:J:93:VAL:HG13  | 35:J:110:MET:HE1  | 1.79                     | 0.65              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 36:K:18:VAL:CG1   | 36:K:19:PRO:HD3  | 2.27                     | 0.65              |
| 51:Z:6:ARG:C      | 51:Z:8:ASN:H     | 2.04                     | 0.65              |
| 53:3:731:G:O2'    | 53:3:732:C:H5'   | 1.96                     | 0.65              |
| 54:1:2241:A:H2'   | 54:1:2242:G:H8   | 1.61                     | 0.65              |
| 59:8:503:GLY:HA3  | 59:8:600:ALA:HB2 | 1.79                     | 0.65              |
| 3:d:137:LYS:O     | 3:d:141:MET:HG3  | 1.96                     | 0.65              |
| 21:v:47:VAL:HG22  | 21:v:50:MET:HE2  | 1.79                     | 0.65              |
| 39:N:83:THR:HG23  | 39:N:97:LEU:HD23 | 1.79                     | 0.65              |
| 44:S:74:ARG:HB3   | 53:3:1358:U:OP1  | 1.97                     | 0.65              |
| 53:3:1513:A:H2'   | 53:3:1514:G:H8   | 1.61                     | 0.65              |
| 54:1:1179:G:C5    | 54:1:1180:U:H1'  | 2.31                     | 0.65              |
| 54:1:1965:C:H5''  | 54:1:1966:A:H2'  | 1.77                     | 0.65              |
| 59:8:566:LEU:HD22 | 59:8:610:PRO:HB2 | 1.79                     | 0.65              |
| 5:f:140:ILE:HG13  | 5:f:141:GLY:N    | 2.12                     | 0.64              |
| 9:j:1:MET:HE3     | 9:j:2:LYS:N      | 2.12                     | 0.64              |
| 14:o:62:LEU:HD22  | 14:o:70:ALA:HB1  | 1.79                     | 0.64              |
| 26:A:15:SER:HA    | 26:A:21:VAL:HG13 | 1.77                     | 0.64              |
| 43:R:97:ARG:H     | 53:3:1307:U:H3'  | 1.61                     | 0.64              |
| 53:3:1164:G:H22   | 53:3:1171:A:N6   | 1.93                     | 0.64              |
| 4:e:116:LEU:HG    | 4:e:117:SER:H    | 1.62                     | 0.64              |
| 14:o:34:HIS:HA    | 14:o:53:THR:OG1  | 1.98                     | 0.64              |
| 21:v:76:ASP:HB3   | 21:v:90:ASP:HB2  | 1.79                     | 0.64              |
| 25:z:5:LYS:HB2    | 25:z:57:GLU:HG2  | 1.78                     | 0.64              |
| 33:H:110:LEU:HD13 | 33:H:203:LYS:NZ  | 2.12                     | 0.64              |
| 53:3:884:U:H4'    | 53:3:885:G:H5''  | 1.79                     | 0.64              |
| 53:3:1014:A:H2'   | 53:3:1015:G:O4'  | 1.97                     | 0.64              |
| 54:1:813:U:H2'    | 54:1:814:C:H6    | 1.61                     | 0.64              |
| 59:8:550:ILE:HB   | 59:8:551:PRO:HD3 | 1.77                     | 0.64              |
| 8:i:52:LEU:HB2    | 8:i:54:ILE:HD11  | 1.78                     | 0.64              |
| 41:P:14:GLN:CD    | 41:P:14:GLN:H    | 2.05                     | 0.64              |
| 54:1:2193:G:H2'   | 54:1:2194:U:C6   | 2.33                     | 0.64              |
| 59:8:63:ILE:HG23  | 59:8:95:PHE:CE1  | 2.33                     | 0.64              |
| 53:3:715:A:H2'    | 53:3:716:A:C8    | 2.31                     | 0.64              |
| 2:c:201:LEU:C     | 2:c:202:ILE:HD12 | 2.22                     | 0.64              |
| 30:E:5:THR:HG23   | 30:E:61:LEU:HA   | 1.78                     | 0.64              |
| 35:J:57:ALA:O     | 35:J:61:LYS:HD3  | 1.98                     | 0.64              |
| 36:K:39:LEU:O     | 36:K:39:LEU:HD23 | 1.97                     | 0.64              |
| 38:M:64:TYR:CD1   | 38:M:69:ALA:HB2  | 2.33                     | 0.64              |
| 53:3:15:G:N1      | 53:3:1080:A:H1'  | 2.11                     | 0.64              |
| 54:1:1821:A:H2'   | 54:1:1822:C:C6   | 2.33                     | 0.64              |
| 56:5:26:A:H61     | 56:5:44:G:H1     | 0.84                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 59:8:498:VAL:HG23 | 59:8:607:LYS:HD2  | 1.77                     | 0.64              |
| 11:l:69:ARG:HD3   | 54:1:2406:A:N3    | 2.12                     | 0.64              |
| 14:o:62:LEU:HD21  | 14:o:65:THR:HG22  | 1.79                     | 0.64              |
| 29:D:4:THR:HG22   | 54:1:687:C:H1'    | 1.80                     | 0.64              |
| 32:G:212:TYR:O    | 32:G:216:VAL:HG23 | 1.97                     | 0.64              |
| 34:I:28:ASP:O     | 34:I:30:LYS:HG2   | 1.97                     | 0.64              |
| 35:J:19:ARG:HB3   | 35:J:32:PHE:CE1   | 2.33                     | 0.64              |
| 36:K:51:ILE:C     | 36:K:53:LYS:H     | 2.03                     | 0.64              |
| 42:Q:77:SER:HA    | 42:Q:102:ASP:OD2  | 1.96                     | 0.64              |
| 43:R:49:GLU:O     | 43:R:52:ILE:HG22  | 1.98                     | 0.64              |
| 43:R:85:TYR:HB3   | 49:X:72:GLU:OE2   | 1.97                     | 0.64              |
| 54:1:687:C:H6     | 54:1:687:C:H5'    | 1.60                     | 0.64              |
| 59:8:474:LYS:HA   | 59:8:479:VAL:H    | 1.63                     | 0.64              |
| 16:q:16:ILE:HG13  | 16:q:31:TYR:HE1   | 1.63                     | 0.64              |
| 30:E:30:HIS:O     | 30:E:32:LEU:HG    | 1.98                     | 0.64              |
| 30:E:30:HIS:C     | 30:E:32:LEU:H     | 2.05                     | 0.64              |
| 32:G:160:LEU:HB3  | 32:G:182:VAL:HG12 | 1.79                     | 0.64              |
| 35:J:81:GLN:H     | 35:J:146:MET:CE   | 2.10                     | 0.64              |
| 47:V:29:LYS:HB2   | 47:V:36:PHE:CE1   | 2.31                     | 0.64              |
| 49:X:57:VAL:HG11  | 49:X:75:PRO:HD2   | 1.78                     | 0.64              |
| 54:1:849:A:H2'    | 54:1:850:U:C6     | 2.33                     | 0.64              |
| 54:1:1564:C:H2'   | 54:1:1565:C:O4'   | 1.96                     | 0.64              |
| 54:1:1773:A:C2'   | 54:1:1774:C:H5'   | 2.28                     | 0.64              |
| 37:L:24:LYS:O     | 37:L:28:ILE:HG13  | 1.98                     | 0.64              |
| 44:S:85:GLU:OE2   | 44:S:86:ALA:HB2   | 1.97                     | 0.64              |
| 54:1:2183:A:H2'   | 54:1:2184:A:C8    | 2.32                     | 0.64              |
| 59:8:183:VAL:HA   | 59:8:190:ALA:HA   | 1.80                     | 0.64              |
| 9:j:49:ASP:OD2    | 9:j:121:LYS:HE2   | 1.98                     | 0.64              |
| 15:p:3:ILE:H      | 15:p:3:ILE:CD1    | 2.08                     | 0.64              |
| 40:O:44:THR:HG21  | 40:O:70:HIS:ND1   | 2.11                     | 0.64              |
| 44:S:27:LYS:HD2   | 44:S:27:LYS:C     | 2.23                     | 0.64              |
| 46:U:5:ARG:HH12   | 46:U:22:ALA:HB3   | 1.63                     | 0.64              |
| 48:W:33:THR:HG22  | 48:W:37:LYS:N     | 2.10                     | 0.64              |
| 53:3:1302:C:O2'   | 53:3:1303:C:H5'   | 1.96                     | 0.64              |
| 53:3:1355:G:O2'   | 53:3:1356:G:H5'   | 1.97                     | 0.64              |
| 59:8:267:GLY:HA3  | 59:8:274:GLY:HA3  | 1.80                     | 0.64              |
| 9:j:120:ARG:HH21  | 9:j:120:ARG:HG3   | 1.62                     | 0.64              |
| 26:A:8:LYS:HB2    | 26:A:10:GLU:OE1   | 1.97                     | 0.64              |
| 40:O:41:PRO:HD2   | 53:3:1150:A:C2    | 2.33                     | 0.64              |
| 43:R:24:VAL:HG12  | 43:R:28:ARG:CD    | 2.28                     | 0.64              |
| 53:3:64:G:H4'     | 53:3:65:A:H5''    | 1.80                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:3:1506:U:O2'  | 53:3:1507:A:H5'   | 1.98                     | 0.64              |
| 54:1:198:C:O2'   | 54:1:199:A:H5'    | 1.97                     | 0.64              |
| 54:1:437:U:H2'   | 54:1:438:G:C8     | 2.33                     | 0.64              |
| 54:1:947:A:H2'   | 54:1:948:C:H6     | 1.62                     | 0.64              |
| 54:1:2327:A:H2'  | 54:1:2328:A:C8    | 2.32                     | 0.64              |
| 59:8:170:GLN:HB3 | 59:8:265:THR:HA   | 1.80                     | 0.64              |
| 59:8:173:ILE:HA  | 59:8:211:MET:HE1  | 1.80                     | 0.64              |
| 8:i:48:ILE:HG13  | 8:i:49:GLU:N      | 2.12                     | 0.63              |
| 21:v:20:LEU:HD11 | 21:v:27:PRO:HD3   | 1.79                     | 0.63              |
| 40:O:73:LEU:HD11 | 53:3:1124:G:C5'   | 2.27                     | 0.63              |
| 42:Q:49:ARG:HG2  | 42:Q:49:ARG:HH11  | 1.61                     | 0.63              |
| 53:3:193:C:H2'   | 53:3:194:C:C6     | 2.33                     | 0.63              |
| 12:m:35:ALA:HB2  | 12:m:102:LEU:HD21 | 1.80                     | 0.63              |
| 34:I:59:LYS:O    | 34:I:63:ILE:HG13  | 1.98                     | 0.63              |
| 35:J:79:THR:HB   | 35:J:121:ASN:OD1  | 1.99                     | 0.63              |
| 43:R:98:GLY:HA3  | 53:3:1307:U:O5'   | 1.98                     | 0.63              |
| 53:3:56:U:H2'    | 53:3:57:G:H8      | 1.61                     | 0.63              |
| 53:3:78:A:H2'    | 53:3:79:G:O4'     | 1.99                     | 0.63              |
| 53:3:744:C:H2'   | 53:3:745:G:H8     | 1.63                     | 0.63              |
| 53:3:962:C:H1'   | 53:3:1201:A:N6    | 2.13                     | 0.63              |
| 59:8:282:VAL:HA  | 59:8:286:LEU:HD13 | 1.80                     | 0.63              |
| 4:e:33:ILE:HG12  | 4:e:95:MET:HG3    | 1.80                     | 0.63              |
| 16:q:111:LYS:HG2 | 17:r:48:LYS:HZ1   | 1.64                     | 0.63              |
| 53:3:1066:C:H2'  | 53:3:1066:C:O2    | 1.96                     | 0.63              |
| 54:1:2834:G:H2'  | 54:1:2879:A:H61   | 1.63                     | 0.63              |
| 55:2:65:U:H3'    | 55:2:108:A:N6     | 2.12                     | 0.63              |
| 59:8:170:GLN:HB2 | 59:8:265:THR:HG22 | 1.81                     | 0.63              |
| 23:x:35:HIS:CG   | 23:x:36:ARG:H     | 2.17                     | 0.63              |
| 30:E:57:VAL:HG12 | 30:E:61:LEU:HD11  | 1.80                     | 0.63              |
| 32:G:131:LYS:HG3 | 53:3:1158:C:O2'   | 1.98                     | 0.63              |
| 40:O:36:VAL:HG22 | 53:3:1123:U:H4'   | 1.80                     | 0.63              |
| 41:P:22:ILE:HB   | 41:P:85:VAL:HA    | 1.80                     | 0.63              |
| 43:R:97:ARG:HB3  | 53:3:1307:U:C4    | 2.33                     | 0.63              |
| 53:3:224:U:H2'   | 53:3:225:C:C6     | 2.32                     | 0.63              |
| 53:3:1066:C:H5'  | 53:3:1067:A:OP2   | 1.97                     | 0.63              |
| 54:1:1103:A:H3'  | 54:1:1104:C:H6    | 1.62                     | 0.63              |
| 54:1:1779:U:H5   | 54:1:1784:A:N7    | 1.96                     | 0.63              |
| 59:8:349:VAL:HA  | 59:8:399:ASP:CB   | 2.24                     | 0.63              |
| 39:N:35:GLU:HA   | 39:N:39:GLY:HA3   | 1.79                     | 0.63              |
| 45:T:58:MET:HA   | 45:T:61:GLN:HB3   | 1.81                     | 0.63              |
| 54:1:639:U:H2'   | 54:1:640:C:C6     | 2.34                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 54:1:2691:C:H5'  | 54:1:2872:A:O4'   | 1.99                     | 0.63              |
| 59:8:168:PRO:O   | 59:8:185:LEU:HD12 | 1.99                     | 0.63              |
| 4:e:65:LEU:HD22  | 55:2:42:C:C5      | 2.33                     | 0.63              |
| 10:k:22:ILE:HD11 | 10:k:40:LYS:HG3   | 1.81                     | 0.63              |
| 34:I:12:ARG:HD3  | 34:I:36:ALA:C     | 2.23                     | 0.63              |
| 40:O:22:THR:O    | 40:O:25:ILE:HG22  | 1.98                     | 0.63              |
| 46:U:75:ILE:O    | 46:U:78:VAL:HG12  | 1.98                     | 0.63              |
| 51:Z:39:LYS:N    | 51:Z:40:PRO:HD2   | 2.13                     | 0.63              |
| 53:3:952:U:H5'   | 53:3:972:C:H41    | 1.63                     | 0.63              |
| 54:1:704:G:H1'   | 54:1:727:A:N6     | 2.12                     | 0.63              |
| 54:1:2317:A:H2'  | 54:1:2318:G:O4'   | 1.99                     | 0.63              |
| 57:6:35:A:C2     | 58:4:18:G:C2      | 2.86                     | 0.63              |
| 59:8:425:LYS:O   | 59:8:428:GLN:HB3  | 1.99                     | 0.63              |
| 1:b:180:MET:HE1  | 1:b:268:ARG:NE    | 2.11                     | 0.63              |
| 39:N:25:GLY:HA3  | 39:N:57:VAL:HG13  | 1.79                     | 0.63              |
| 54:1:2692:G:H2'  | 54:1:2693:G:H8    | 1.64                     | 0.63              |
| 59:8:585:ASP:C   | 59:8:587:ASP:H    | 2.06                     | 0.63              |
| 5:f:25:ILE:O     | 5:f:31:GLU:HG3    | 1.99                     | 0.63              |
| 37:L:70:PRO:O    | 37:L:95:ARG:HD3   | 1.99                     | 0.63              |
| 40:O:35:GLN:HG3  | 40:O:78:GLU:HB2   | 1.80                     | 0.63              |
| 42:Q:25:ALA:HA   | 53:3:553:A:O2'    | 1.99                     | 0.63              |
| 43:R:97:ARG:HB2  | 53:3:1307:U:N3    | 2.14                     | 0.63              |
| 53:3:327:A:O2'   | 53:3:328:C:H4'    | 1.98                     | 0.63              |
| 54:1:146:A:H2'   | 54:1:147:C:C6     | 2.34                     | 0.63              |
| 9:j:40:HIS:ND1   | 9:j:41:LYS:HG3    | 2.13                     | 0.63              |
| 10:k:71:ARG:HB3  | 10:k:72:PRO:HD2   | 1.80                     | 0.63              |
| 34:I:202:LEU:O   | 34:I:202:LEU:HD23 | 1.99                     | 0.63              |
| 35:J:80:LEU:HD13 | 35:J:122:VAL:HG13 | 1.81                     | 0.63              |
| 53:3:273:U:C2'   | 53:3:274:A:H5'    | 2.29                     | 0.63              |
| 54:1:1102:C:H2'  | 54:1:1103:A:H8    | 1.64                     | 0.63              |
| 59:8:445:PHE:CE1 | 59:8:458:ILE:HG23 | 2.33                     | 0.63              |
| 2:c:20:VAL:HG12  | 2:c:22:ILE:HG23   | 1.80                     | 0.62              |
| 5:f:139:VAL:O    | 5:f:143:VAL:HG23  | 1.99                     | 0.62              |
| 16:q:60:TRP:O    | 16:q:64:ILE:HG13  | 1.99                     | 0.62              |
| 29:D:12:ARG:NE   | 29:D:44:VAL:HG21  | 2.14                     | 0.62              |
| 32:G:207:ARG:HD2 | 32:G:207:ARG:C    | 2.24                     | 0.62              |
| 42:Q:56:LEU:HD12 | 42:Q:56:LEU:N     | 2.14                     | 0.62              |
| 44:S:80:ARG:O    | 44:S:83:VAL:HG12  | 1.98                     | 0.62              |
| 53:3:1363:A:H2'  | 53:3:1365:G:N7    | 2.13                     | 0.62              |
| 54:1:554:U:H2'   | 54:1:555:G:O4'    | 1.99                     | 0.62              |
| 54:1:864:G:O2'   | 54:1:865:C:H5'    | 1.99                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 54:1:1779:U:C5   | 54:1:1784:A:N7    | 2.67                     | 0.62              |
| 54:1:2452:C:H42  | 54:1:2504:U:H3    | 1.45                     | 0.62              |
| 59:8:104:ARG:HG3 | 59:8:133:TYR:CD1  | 2.34                     | 0.62              |
| 59:8:530:ASN:ND2 | 59:8:530:ASN:O    | 2.30                     | 0.62              |
| 1:b:77:VAL:HG21  | 1:b:109:LEU:HD21  | 1.80                     | 0.62              |
| 20:u:9:GLU:HG3   | 20:u:72:PHE:HB3   | 1.82                     | 0.62              |
| 41:P:92:ARG:HE   | 51:Z:24:LYS:HZ2   | 1.45                     | 0.62              |
| 59:8:296:ASN:HA  | 59:8:307:ALA:O    | 1.99                     | 0.62              |
| 59:8:559:GLU:OE2 | 59:8:560:GLN:HB2  | 1.99                     | 0.62              |
| 2:c:48:ILE:HG23  | 2:c:84:LEU:HD11   | 1.80                     | 0.62              |
| 33:H:191:THR:O   | 53:3:1206:G:O2'   | 2.13                     | 0.62              |
| 40:O:39:PRO:CB   | 53:3:1123:U:O4    | 2.47                     | 0.62              |
| 42:Q:73:LEU:HD12 | 42:Q:73:LEU:N     | 2.14                     | 0.62              |
| 52:a:21:TYR:CD2  | 52:a:222:VAL:HG13 | 2.34                     | 0.62              |
| 3:d:68:ALA:HA    | 54:1:1255:U:C5    | 2.35                     | 0.62              |
| 7:h:56:ARG:NE    | 7:h:83:ALA:HB2    | 2.12                     | 0.62              |
| 32:G:17:HIS:CG   | 32:G:18:GLN:H     | 2.16                     | 0.62              |
| 40:O:65:TYR:HA   | 44:S:98:ALA:H     | 1.65                     | 0.62              |
| 53:3:15:G:H22    | 53:3:1080:A:H1'   | 1.64                     | 0.62              |
| 54:1:2129:C:H2'  | 54:1:2159:G:H22   | 1.63                     | 0.62              |
| 56:5:30:G:H2'    | 56:5:31:G:C8      | 2.35                     | 0.62              |
| 11:l:23:ILE:H    | 11:l:23:ILE:CD1   | 2.12                     | 0.62              |
| 33:H:149:LYS:NZ  | 33:H:166:TRP:HE3  | 1.96                     | 0.62              |
| 51:Z:32:ARG:HH12 | 51:Z:34:ARG:HD2   | 1.64                     | 0.62              |
| 56:5:2:G:O2'     | 56:5:3:G:H2'      | 2.00                     | 0.62              |
| 4:e:35:LEU:HB3   | 4:e:88:VAL:HB     | 1.81                     | 0.62              |
| 5:f:79:THR:HB    | 5:f:80:GLU:OE1    | 1.99                     | 0.62              |
| 13:n:103:ARG:HB2 | 13:n:110:MET:HE2  | 1.79                     | 0.62              |
| 17:r:15:SER:O    | 17:r:18:GLN:HG2   | 1.99                     | 0.62              |
| 43:R:92:ARG:NH1  | 43:R:92:ARG:HB2   | 2.14                     | 0.62              |
| 52:a:42:VAL:HG21 | 52:a:185:LEU:HD13 | 1.80                     | 0.62              |
| 53:3:1237:C:OP1  | 53:3:1238:A:H1'   | 1.99                     | 0.62              |
| 54:1:1900:A:H1'  | 54:1:1970:A:H2'   | 1.81                     | 0.62              |
| 2:c:149:ASN:O    | 2:c:152:PRO:HD2   | 2.00                     | 0.62              |
| 13:n:12:ARG:HB2  | 13:n:12:ARG:NH2   | 2.15                     | 0.62              |
| 21:v:21:ARG:HA   | 21:v:25:LYS:O     | 2.00                     | 0.62              |
| 43:R:89:ARG:O    | 43:R:94:LEU:HB2   | 1.99                     | 0.62              |
| 44:S:100:TRP:HB3 | 53:3:1115:U:H1'   | 1.82                     | 0.62              |
| 53:3:766:A:H2'   | 53:3:767:A:O4'    | 2.00                     | 0.62              |
| 54:1:419:U:H2'   | 54:1:420:C:C6     | 2.35                     | 0.62              |
| 54:1:1539:U:H2'  | 54:1:1540:G:H8    | 1.62                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:2048:G:C3'   | 54:1:2049:G:H5''  | 2.30                     | 0.62              |
| 54:1:2130:U:H4'   | 54:1:2134:A:H4'   | 1.82                     | 0.62              |
| 54:1:2345:G:N3    | 54:1:2381:A:H2'   | 2.14                     | 0.62              |
| 1:b:143:VAL:HG12  | 1:b:144:GLU:O     | 2.00                     | 0.62              |
| 5:f:8:VAL:O       | 5:f:48:THR:HB     | 1.99                     | 0.62              |
| 8:i:23:VAL:HG13   | 8:i:26:ALA:HB3    | 1.80                     | 0.62              |
| 21:v:82:TYR:CD1   | 21:v:83:LYS:HG3   | 2.34                     | 0.62              |
| 45:T:31:LEU:O     | 45:T:35:ILE:HG13  | 1.99                     | 0.62              |
| 46:U:35:ARG:HH22  | 46:U:38:PHE:HB3   | 1.64                     | 0.62              |
| 53:3:147:G:H2'    | 53:3:148:G:C8     | 2.34                     | 0.62              |
| 53:3:529:G:H4'    | 53:3:533:A:C2     | 2.34                     | 0.62              |
| 54:1:100:U:H4'    | 54:1:101:A:O4'    | 2.00                     | 0.62              |
| 54:1:281:C:H42    | 54:1:359:G:H1     | 1.47                     | 0.62              |
| 10:k:30:ARG:HG2   | 54:1:2674:G:H4'   | 1.81                     | 0.62              |
| 14:o:107:ALA:HB1  | 14:o:111:ARG:HH22 | 1.65                     | 0.62              |
| 23:x:35:HIS:HB2   | 23:x:55:MET:HE1   | 1.80                     | 0.62              |
| 30:E:18:LYS:HG3   | 54:1:651:G:H5'    | 1.81                     | 0.62              |
| 35:J:104:ILE:HG23 | 35:J:111:ARG:HH12 | 1.64                     | 0.62              |
| 36:K:66:ALA:HB1   | 36:K:67:PRO:HD2   | 1.81                     | 0.62              |
| 37:L:22:LEU:O     | 37:L:26:VAL:HG23  | 1.99                     | 0.62              |
| 43:R:98:GLY:N     | 53:3:1308:U:OP2   | 2.32                     | 0.62              |
| 45:T:45:HIS:O     | 45:T:47:LYS:N     | 2.33                     | 0.62              |
| 53:3:131:A:H2'    | 53:3:132:C:C6     | 2.34                     | 0.62              |
| 10:k:88:ASN:HD22  | 10:k:89:ASN:H     | 1.47                     | 0.62              |
| 39:N:97:LEU:O     | 39:N:101:GLY:N    | 2.33                     | 0.62              |
| 40:O:44:THR:CG2   | 40:O:70:HIS:HA    | 2.29                     | 0.62              |
| 59:8:67:ALA:HA    | 59:8:87:ILE:HA    | 1.81                     | 0.62              |
| 26:A:20:ASN:ND2   | 26:A:39:LYS:HD2   | 2.13                     | 0.61              |
| 30:E:41:ARG:HG3   | 30:E:44:ARG:NH1   | 2.14                     | 0.61              |
| 32:G:67:LEU:HD22  | 32:G:157:PRO:HG2  | 1.82                     | 0.61              |
| 33:H:63:ILE:HG23  | 33:H:98:ALA:HA    | 1.82                     | 0.61              |
| 33:H:178:ARG:HB3  | 33:H:178:ARG:HH11 | 1.65                     | 0.61              |
| 53:3:422:C:H5'    | 53:3:423:G:C2     | 2.34                     | 0.61              |
| 54:1:1441:G:H2'   | 54:1:1442:U:C6    | 2.34                     | 0.61              |
| 55:2:2:G:C6       | 55:2:119:A:N6     | 2.68                     | 0.61              |
| 59:8:11:ARG:HB2   | 59:8:84:ILE:HG13  | 1.81                     | 0.61              |
| 59:8:420:VAL:HG23 | 59:8:431:MET:HE1  | 1.81                     | 0.61              |
| 13:n:10:LEU:HB3   | 13:n:12:ARG:HH22  | 1.65                     | 0.61              |
| 23:x:29:LEU:HD12  | 54:1:2230:G:H5''  | 1.81                     | 0.61              |
| 27:B:16:ARG:HA    | 27:B:19:ASP:OD2   | 1.99                     | 0.61              |
| 29:D:35:ARG:NH1   | 29:D:35:ARG:HB2   | 2.16                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:P:86:LYS:CG    | 41:P:112:VAL:HG23 | 2.30                     | 0.61              |
| 52:a:220:ALA:HA   | 54:1:2176:A:H5'   | 1.82                     | 0.61              |
| 53:3:531:U:C4'    | 53:3:532:A:H5'    | 2.30                     | 0.61              |
| 53:3:919:A:O5'    | 53:3:919:A:H8     | 1.83                     | 0.61              |
| 53:3:945:G:O6     | 53:3:1236:A:N1    | 2.33                     | 0.61              |
| 53:3:1053:G:O2'   | 53:3:1199:U:H5    | 1.82                     | 0.61              |
| 53:3:1060:U:H2'   | 53:3:1061:G:H5'   | 1.82                     | 0.61              |
| 53:3:1121:U:H3    | 53:3:1152:A:H61   | 1.49                     | 0.61              |
| 8:i:21:PRO:HB2    | 8:i:22:PRO:HD3    | 1.82                     | 0.61              |
| 33:H:5:HIS:CE1    | 33:H:7:ASN:HB3    | 2.35                     | 0.61              |
| 34:I:96:ARG:HB3   | 34:I:98:ASP:OD1   | 2.00                     | 0.61              |
| 40:O:39:PRO:CB    | 53:3:1123:U:C4    | 2.83                     | 0.61              |
| 45:T:64:LYS:HE2   | 53:3:581:G:H5''   | 1.82                     | 0.61              |
| 53:3:1121:U:H2'   | 53:3:1122:U:C6    | 2.35                     | 0.61              |
| 53:3:1234:C:H1'   | 53:3:1364:U:O2    | 2.00                     | 0.61              |
| 53:3:1241:G:H2'   | 53:3:1242:G:H8    | 1.66                     | 0.61              |
| 54:1:608:A:H2'    | 54:1:609:A:C8     | 2.36                     | 0.61              |
| 54:1:2323:G:H2'   | 54:1:2324:U:O4'   | 2.00                     | 0.61              |
| 59:8:9:ARG:HD2    | 59:8:81:PRO:O     | 2.01                     | 0.61              |
| 59:8:189:LYS:HE3  | 59:8:204:TYR:CE1  | 2.35                     | 0.61              |
| 59:8:540:ILE:HG13 | 59:8:545:ILE:HD12 | 1.82                     | 0.61              |
| 1:b:207:ALA:HB2   | 54:1:1790:C:O2'   | 2.00                     | 0.61              |
| 4:e:73:VAL:HG12   | 4:e:75:GLY:H      | 1.66                     | 0.61              |
| 8:i:27:LEU:HD23   | 8:i:27:LEU:H      | 1.64                     | 0.61              |
| 11:l:19:LEU:HD23  | 54:1:587:C:C2     | 2.35                     | 0.61              |
| 18:s:29:VAL:HG21  | 18:s:69:LEU:HB3   | 1.82                     | 0.61              |
| 38:M:64:TYR:HA    | 38:M:69:ALA:HA    | 1.81                     | 0.61              |
| 53:3:513:C:H2'    | 53:3:514:C:C6     | 2.35                     | 0.61              |
| 53:3:1371:G:H2'   | 53:3:1372:U:H6    | 1.65                     | 0.61              |
| 53:3:1441:A:H2'   | 53:3:1442:G:H5'   | 1.83                     | 0.61              |
| 54:1:1744:A:H3'   | 54:1:1745:A:H8    | 1.64                     | 0.61              |
| 59:8:523:TYR:HB2  | 59:8:577:ARG:HH12 | 1.65                     | 0.61              |
| 1:b:16:VAL:HB     | 1:b:203:VAL:HG22  | 1.82                     | 0.61              |
| 5:f:9:VAL:HA      | 5:f:48:THR:HB     | 1.81                     | 0.61              |
| 5:f:85:LYS:HG3    | 5:f:131:VAL:HG22  | 1.82                     | 0.61              |
| 17:r:39:LEU:O     | 17:r:49:ILE:HG23  | 2.00                     | 0.61              |
| 22:w:15:LYS:HB2   | 22:w:17:LEU:HD11  | 1.81                     | 0.61              |
| 33:H:42:LEU:HD23  | 33:H:54:ILE:CD1   | 2.29                     | 0.61              |
| 46:U:36:VAL:HG23  | 46:U:53:ASP:OD1   | 2.00                     | 0.61              |
| 53:3:56:U:H2'     | 53:3:57:G:C8      | 2.36                     | 0.61              |
| 53:3:537:G:H5'    | 53:3:537:G:H8     | 1.63                     | 0.61              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 53:3:908:A:H2'    | 53:3:909:A:H8    | 1.64                     | 0.61              |
| 53:3:1507:A:H2'   | 53:3:1508:A:C8   | 2.36                     | 0.61              |
| 54:1:202:U:H2'    | 54:1:203:A:O4'   | 2.00                     | 0.61              |
| 54:1:1300:G:C4'   | 54:1:1301:A:H5'' | 2.31                     | 0.61              |
| 54:1:2193:G:H2'   | 54:1:2194:U:H6   | 1.65                     | 0.61              |
| 54:1:2331:G:H2'   | 54:1:2332:C:C6   | 2.36                     | 0.61              |
| 59:8:438:LEU:HD22 | 59:8:473:MET:SD  | 2.41                     | 0.61              |
| 11:l:9:ALA:HB3    | 11:l:12:SER:HB2  | 1.82                     | 0.61              |
| 13:n:28:LEU:HD23  | 13:n:48:VAL:HG21 | 1.82                     | 0.61              |
| 26:A:36:VAL:HB    | 26:A:41:HIS:HB2  | 1.82                     | 0.61              |
| 35:J:55:VAL:HG23  | 35:J:56:PRO:HD3  | 1.83                     | 0.61              |
| 52:a:172:HIS:HB3  | 54:1:2123:G:H4'  | 1.83                     | 0.61              |
| 53:3:697:U:H2'    | 53:3:698:G:H5'   | 1.82                     | 0.61              |
| 53:3:866:C:H4'    | 53:3:919:A:C5'   | 2.27                     | 0.61              |
| 53:3:1410:A:H2'   | 53:3:1411:C:C6   | 2.36                     | 0.61              |
| 54:1:1802:A:H2'   | 54:1:1803:A:C8   | 2.36                     | 0.61              |
| 54:1:2167:U:H3    | 54:1:2170:A:N6   | 1.98                     | 0.61              |
| 58:4:11:U:H2'     | 58:4:12:A:O4'    | 2.00                     | 0.61              |
| 11:l:70:LYS:O     | 11:l:73:ILE:HG12 | 2.01                     | 0.61              |
| 13:n:29:VAL:HG12  | 13:n:78:LYS:HD3  | 1.82                     | 0.61              |
| 30:E:31:ILE:CD1   | 54:1:2391:G:H5'  | 2.30                     | 0.61              |
| 35:J:21:SER:HB2   | 53:3:15:G:H21    | 1.65                     | 0.61              |
| 37:L:36:SER:HB3   | 39:N:42:THR:HG21 | 1.82                     | 0.61              |
| 42:Q:38:THR:HG21  | 42:Q:48:LEU:HG   | 1.83                     | 0.61              |
| 46:U:67:ILE:H     | 46:U:67:ILE:HD12 | 1.66                     | 0.61              |
| 48:W:15:GLU:OE1   | 53:3:845:A:H5''  | 2.01                     | 0.61              |
| 53:3:15:G:N2      | 53:3:1080:A:H1'  | 2.15                     | 0.61              |
| 53:3:580:C:H2'    | 53:3:581:G:O4'   | 2.00                     | 0.61              |
| 53:3:936:C:C1'    | 53:3:1383:C:H41  | 2.14                     | 0.61              |
| 54:1:594:U:H2'    | 54:1:595:C:C6    | 2.36                     | 0.61              |
| 54:1:2861:U:H2'   | 54:1:2862:G:H8   | 1.65                     | 0.61              |
| 59:8:147:MET:HA   | 59:8:176:GLU:CD  | 2.26                     | 0.61              |
| 10:k:108:ARG:HG3  | 10:k:113:MET:HE1 | 1.83                     | 0.61              |
| 19:t:91:GLN:H     | 19:t:91:GLN:CD   | 2.09                     | 0.61              |
| 23:x:69:GLU:HA    | 23:x:72:ALA:HB3  | 1.82                     | 0.61              |
| 43:R:2:ARG:O      | 43:R:52:ILE:HD11 | 2.01                     | 0.61              |
| 50:Y:43:LYS:HE3   | 50:Y:85:LEU:HD23 | 1.81                     | 0.61              |
| 54:1:662:G:O2'    | 54:1:663:G:H5'   | 2.00                     | 0.61              |
| 54:1:1026:G:H2'   | 54:1:1027:A:H8   | 1.66                     | 0.61              |
| 54:1:1935:G:H1'   | 54:1:1964:G:N2   | 2.16                     | 0.61              |
| 57:6:35:A:C2      | 58:4:18:G:N2     | 2.69                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 59:8:498:VAL:CG1 | 59:8:522:MET:HG2  | 2.31                     | 0.61              |
| 11:l:93:ASN:C    | 11:l:95:LEU:H     | 2.07                     | 0.61              |
| 12:m:12:MET:CA   | 54:1:910:A:H62    | 2.08                     | 0.61              |
| 21:v:4:ILE:HB    | 21:v:63:ILE:HD12  | 1.83                     | 0.61              |
| 53:3:114:U:O2'   | 53:3:115:G:H5'    | 2.01                     | 0.61              |
| 54:1:2221:G:O2'  | 54:1:2222:C:H5'   | 2.00                     | 0.61              |
| 59:8:54:GLU:HG3  | 59:8:55:GLN:HE21  | 1.66                     | 0.61              |
| 59:8:171:LEU:HB3 | 59:8:183:VAL:CG1  | 2.31                     | 0.61              |
| 11:l:8:PRO:HD3   | 54:1:1244:A:H5'   | 1.83                     | 0.61              |
| 33:H:115:VAL:O   | 33:H:119:ILE:HG13 | 2.00                     | 0.61              |
| 36:K:3:HIS:CG    | 36:K:95:ALA:HB2   | 2.36                     | 0.61              |
| 51:Z:49:ALA:O    | 51:Z:53:LYS:HG3   | 2.01                     | 0.61              |
| 53:3:662:U:H2'   | 53:3:663:A:C8     | 2.35                     | 0.61              |
| 53:3:1014:A:C2   | 53:3:1219:A:H1'   | 2.36                     | 0.61              |
| 53:3:1148:U:C3'  | 53:3:1149:C:H4'   | 2.26                     | 0.61              |
| 54:1:310:A:C2'   | 54:1:311:A:H5''   | 2.31                     | 0.61              |
| 54:1:1300:G:H4'  | 54:1:1301:A:H5'   | 1.83                     | 0.61              |
| 54:1:1645:G:H5'' | 54:1:1646:C:H5'   | 1.83                     | 0.61              |
| 54:1:2277:G:C3'  | 54:1:2278:A:H5''  | 2.31                     | 0.61              |
| 59:8:410:GLU:HG3 | 59:8:443:PRO:HB2  | 1.81                     | 0.61              |
| 21:v:75:GLN:HB3  | 21:v:90:ASP:O     | 2.01                     | 0.60              |
| 32:G:135:MET:HA  | 32:G:138:ARG:HB3  | 1.82                     | 0.60              |
| 50:Y:34:VAL:HG21 | 50:Y:53:MET:HG2   | 1.82                     | 0.60              |
| 53:3:298:A:H2'   | 53:3:299:G:O4'    | 2.01                     | 0.60              |
| 54:1:1022:G:H22  | 54:1:1142:A:H2    | 1.48                     | 0.60              |
| 55:2:2:G:O6      | 55:2:119:A:N6     | 2.33                     | 0.60              |
| 2:c:31:ALA:O     | 2:c:33:ARG:HD3    | 2.01                     | 0.60              |
| 11:l:79:LEU:HG   | 11:l:111:ILE:O    | 2.00                     | 0.60              |
| 13:n:63:ARG:HH22 | 54:1:1454:C:H5'   | 1.63                     | 0.60              |
| 15:p:28:LYS:HB3  | 15:p:39:LEU:HD11  | 1.83                     | 0.60              |
| 34:I:95:GLY:O    | 34:I:136:VAL:HG23 | 2.01                     | 0.60              |
| 43:R:97:ARG:CB   | 53:3:1307:U:N3    | 2.64                     | 0.60              |
| 53:3:1005:A:H2'  | 53:3:1006:G:O4'   | 2.00                     | 0.60              |
| 54:1:226:A:H2'   | 54:1:227:A:O4'    | 2.01                     | 0.60              |
| 54:1:437:U:H2'   | 54:1:438:G:H8     | 1.65                     | 0.60              |
| 54:1:1713:A:H61  | 54:1:1745:A:H61   | 1.49                     | 0.60              |
| 55:2:119:A:N3    | 55:2:120:A:H1'    | 2.16                     | 0.60              |
| 2:c:148:GLN:HB2  | 2:c:152:PRO:HG3   | 1.83                     | 0.60              |
| 6:g:9:VAL:HG13   | 6:g:11:ASN:H      | 1.65                     | 0.60              |
| 26:A:62:LYS:HZ3  | 49:X:17:LYS:HA    | 1.67                     | 0.60              |
| 53:3:472:U:H2'   | 53:3:473:U:C6     | 2.36                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:674:G:H2'    | 53:3:675:A:H8     | 1.65                     | 0.60              |
| 54:1:1932:A:H2'   | 54:1:1933:G:O4'   | 2.01                     | 0.60              |
| 59:8:504:LYS:HB2  | 59:8:517:HIS:ND1  | 2.15                     | 0.60              |
| 32:G:99:MET:HG3   | 32:G:100:LEU:HD12 | 1.83                     | 0.60              |
| 35:J:98:ALA:HB2   | 35:J:123:LEU:HG   | 1.83                     | 0.60              |
| 51:Z:9:GLU:CB     | 51:Z:10:PRO:HD3   | 2.30                     | 0.60              |
| 53:3:1398:A:H5''  | 53:3:1398:A:H8    | 1.65                     | 0.60              |
| 54:1:1188:U:O2'   | 54:1:1189:A:H5'   | 2.00                     | 0.60              |
| 59:8:16:SER:O     | 59:8:111:MET:HA   | 2.01                     | 0.60              |
| 59:8:584:HIS:O    | 59:8:585:ASP:C    | 2.40                     | 0.60              |
| 4:e:144:LYS:HG3   | 4:e:145:VAL:HG13  | 1.83                     | 0.60              |
| 10:k:71:ARG:NH2   | 10:k:105:ARG:HB2  | 2.15                     | 0.60              |
| 30:E:1:PRO:HG2    | 54:1:591:U:H1'    | 1.82                     | 0.60              |
| 34:I:62:ARG:HH11  | 34:I:62:ARG:HG3   | 1.66                     | 0.60              |
| 36:K:17:GLN:NE2   | 36:K:20:GLY:HA3   | 2.15                     | 0.60              |
| 48:W:34:GLU:HB3   | 51:Z:18:PHE:CE1   | 2.36                     | 0.60              |
| 53:3:1304:G:H2'   | 53:3:1305:G:C1'   | 2.32                     | 0.60              |
| 54:1:548:G:H2'    | 54:1:549:G:O4'    | 2.01                     | 0.60              |
| 54:1:1746:A:H2'   | 54:1:1747:U:C6    | 2.36                     | 0.60              |
| 54:1:2073:C:O2'   | 54:1:2074:U:H5'   | 2.02                     | 0.60              |
| 56:5:30:G:H2'     | 56:5:31:G:H8      | 1.66                     | 0.60              |
| 59:8:213:GLU:HG2  | 59:8:214:LEU:N    | 2.15                     | 0.60              |
| 8:i:52:LEU:O      | 8:i:54:ILE:HD12   | 2.02                     | 0.60              |
| 22:w:55:LEU:HD12  | 22:w:76:ILE:HD12  | 1.82                     | 0.60              |
| 34:I:96:ARG:NE    | 34:I:133:SER:HA   | 2.15                     | 0.60              |
| 34:I:104:MET:SD   | 34:I:170:LEU:HD22 | 2.41                     | 0.60              |
| 39:N:17:ARG:HH12  | 53:3:1129:C:H4'   | 1.65                     | 0.60              |
| 45:T:88:ARG:H     | 45:T:88:ARG:CD    | 2.15                     | 0.60              |
| 54:1:705:A:H2'    | 54:1:706:A:H8     | 1.66                     | 0.60              |
| 54:1:2141:G:H2'   | 54:1:2142:A:H8    | 1.67                     | 0.60              |
| 59:8:322:PHE:HD1  | 59:8:322:PHE:H    | 1.49                     | 0.60              |
| 15:p:91:VAL:HG21  | 15:p:96:LEU:HD11  | 1.81                     | 0.60              |
| 37:L:50:ALA:HB2   | 37:L:57:GLU:CG    | 2.31                     | 0.60              |
| 43:R:95:PRO:HB3   | 53:3:1307:U:O3'   | 2.01                     | 0.60              |
| 44:S:50:LEU:HB3   | 44:S:51:PRO:HD2   | 1.83                     | 0.60              |
| 44:S:66:THR:HB    | 53:3:1202:U:O2'   | 2.02                     | 0.60              |
| 53:3:396:C:H2'    | 53:3:397:A:H5''   | 1.83                     | 0.60              |
| 53:3:1200:C:H5''  | 53:3:1201:A:C2'   | 2.32                     | 0.60              |
| 53:3:1530:G:H2'   | 53:3:1531:A:C8    | 2.37                     | 0.60              |
| 54:1:2312:U:O2'   | 54:1:2313:C:H5'   | 2.00                     | 0.60              |
| 59:8:343:VAL:HG21 | 59:8:347:ASP:HB2  | 1.84                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 59:8:584:HIS:O   | 59:8:585:ASP:O    | 2.18                     | 0.60              |
| 9:j:40:HIS:HE1   | 9:j:41:LYS:HE3    | 1.66                     | 0.60              |
| 12:m:42:THR:OG1  | 12:m:45:GLN:HG3   | 2.02                     | 0.60              |
| 14:o:25:ARG:HB2  | 14:o:93:ASP:HB2   | 1.82                     | 0.60              |
| 17:r:49:ILE:HB   | 17:r:51:VAL:O     | 2.02                     | 0.60              |
| 38:M:12:ARG:CZ   | 53:3:826:C:H5'    | 2.32                     | 0.60              |
| 51:Z:67:THR:OXT  | 53:3:1167:A:N7    | 2.35                     | 0.60              |
| 53:3:1304:G:O3'  | 53:3:1305:G:O4'   | 2.20                     | 0.60              |
| 54:1:275:C:H2'   | 54:1:276:U:H4'    | 1.84                     | 0.60              |
| 17:r:75:VAL:HG22 | 17:r:86:GLN:OE1   | 2.02                     | 0.60              |
| 21:v:77:VAL:HG23 | 21:v:89:ILE:HG12  | 1.83                     | 0.60              |
| 41:P:86:LYS:HG2  | 41:P:112:VAL:HG23 | 1.84                     | 0.60              |
| 50:Y:43:LYS:HB2  | 50:Y:86:ALA:HB2   | 1.83                     | 0.60              |
| 59:8:94:ASP:OD2  | 59:8:464:LEU:HB2  | 2.02                     | 0.60              |
| 9:j:37:ARG:HG3   | 9:j:118:MET:HE1   | 1.83                     | 0.60              |
| 13:n:12:ARG:HD3  | 13:n:16:HIS:NE2   | 2.17                     | 0.60              |
| 32:G:22:TRP:HB2  | 32:G:188:THR:O    | 2.01                     | 0.60              |
| 34:I:12:ARG:HD2  | 34:I:37:PRO:HA    | 1.82                     | 0.60              |
| 53:3:716:A:H2'   | 53:3:717:U:C6     | 2.37                     | 0.60              |
| 53:3:1095:U:H5'  | 53:3:1109:C:O2    | 2.01                     | 0.60              |
| 53:3:1273:C:H2'  | 53:3:1274:A:O4'   | 2.02                     | 0.60              |
| 54:1:1213:A:H62  | 54:1:1236:G:H1'   | 1.65                     | 0.60              |
| 54:1:1427:A:H4'  | 54:1:1428:C:O5'   | 2.01                     | 0.60              |
| 54:1:2229:U:H2'  | 54:1:2230:G:H8    | 1.66                     | 0.60              |
| 54:1:2277:G:C2'  | 54:1:2278:A:H5''  | 2.32                     | 0.60              |
| 55:2:48:U:H2'    | 55:2:49:C:C6      | 2.37                     | 0.60              |
| 4:e:39:VAL:HG12  | 4:e:85:GLY:HA2    | 1.84                     | 0.59              |
| 9:j:35:ARG:HA    | 9:j:40:HIS:HD2    | 1.67                     | 0.59              |
| 31:F:23:ILE:HD12 | 31:F:23:ILE:N     | 2.15                     | 0.59              |
| 33:H:133:MET:O   | 33:H:137:VAL:HG23 | 2.02                     | 0.59              |
| 59:8:120:GLN:O   | 59:8:121:PRO:C    | 2.39                     | 0.59              |
| 1:b:62:ARG:NH1   | 1:b:84:PRO:HD2    | 2.17                     | 0.59              |
| 2:c:156:PHE:CD1  | 9:j:81:ILE:HD13   | 2.37                     | 0.59              |
| 13:n:35:LYS:HB2  | 13:n:112:TYR:CE1  | 2.37                     | 0.59              |
| 15:p:3:ILE:HD12  | 15:p:3:ILE:N      | 2.11                     | 0.59              |
| 20:u:65:GLN:OE1  | 54:1:328:U:H4'    | 2.01                     | 0.59              |
| 22:w:19:VAL:HG13 | 22:w:34:VAL:HG22  | 1.84                     | 0.59              |
| 22:w:56:PHE:CZ   | 54:1:2365:G:H4'   | 2.36                     | 0.59              |
| 44:S:48:GLN:HG3  | 53:3:1317:C:C2'   | 2.32                     | 0.59              |
| 48:W:20:ILE:HG22 | 48:W:21:ASP:N     | 2.17                     | 0.59              |
| 51:Z:18:PHE:HA   | 51:Z:21:SER:HB3   | 1.82                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:15:G:H8      | 53:3:1396:A:O2'   | 1.85                     | 0.59              |
| 53:3:63:C:H4'     | 53:3:380:G:H4'    | 1.84                     | 0.59              |
| 53:3:536:C:H2'    | 53:3:537:G:H5'    | 1.84                     | 0.59              |
| 53:3:1513:A:H2'   | 53:3:1514:G:C8    | 2.37                     | 0.59              |
| 56:5:49:G:N2      | 56:5:66:C:H1'     | 2.17                     | 0.59              |
| 1:b:41:GLY:C      | 1:b:42:ARG:HD2    | 2.26                     | 0.59              |
| 7:h:80:THR:HA     | 54:1:1107:G:O2'   | 2.02                     | 0.59              |
| 10:k:35:VAL:HG22  | 10:k:69:VAL:HG12  | 1.84                     | 0.59              |
| 11:l:111:ILE:N    | 11:l:111:ILE:HD12 | 2.17                     | 0.59              |
| 12:m:45:GLN:HE21  | 54:1:2485:G:C5'   | 2.14                     | 0.59              |
| 12:m:45:GLN:NE2   | 54:1:2485:G:H5''  | 2.16                     | 0.59              |
| 39:N:17:ARG:HB2   | 39:N:65:THR:OG1   | 2.02                     | 0.59              |
| 39:N:104:THR:HG22 | 39:N:106:ASP:H    | 1.67                     | 0.59              |
| 43:R:76:ILE:O     | 43:R:80:MET:HG2   | 2.02                     | 0.59              |
| 45:T:1:SER:N      | 45:T:34:GLN:HE22  | 1.99                     | 0.59              |
| 50:Y:85:LEU:HD23  | 50:Y:85:LEU:O     | 2.02                     | 0.59              |
| 54:1:176:A:O2'    | 54:1:177:G:H5'    | 2.02                     | 0.59              |
| 59:8:15:ILE:HD12  | 59:8:86:ILE:HD11  | 1.83                     | 0.59              |
| 59:8:209:ALA:O    | 59:8:212:VAL:HG12 | 2.03                     | 0.59              |
| 59:8:352:SER:HB2  | 59:8:404:ILE:HG23 | 1.85                     | 0.59              |
| 1:b:77:VAL:HG13   | 1:b:91:ALA:HB1    | 1.83                     | 0.59              |
| 32:G:164:ASP:HB2  | 32:G:203:ASP:OD2  | 2.02                     | 0.59              |
| 33:H:96:VAL:HB    | 33:H:97:PRO:HD2   | 1.83                     | 0.59              |
| 36:K:49:TYR:HE1   | 48:W:65:SER:HA    | 1.67                     | 0.59              |
| 40:O:11:LYS:HD3   | 40:O:71:LEU:HG    | 1.84                     | 0.59              |
| 44:S:52:ARG:HG2   | 44:S:58:ARG:NH1   | 2.17                     | 0.59              |
| 45:T:88:ARG:H     | 45:T:88:ARG:HD3   | 1.66                     | 0.59              |
| 53:3:513:C:H2'    | 53:3:514:C:H6     | 1.67                     | 0.59              |
| 54:1:1821:A:H2'   | 54:1:1822:C:H6    | 1.68                     | 0.59              |
| 59:8:323:LYS:HE3  | 59:8:325:ALA:HB2  | 1.85                     | 0.59              |
| 4:e:121:PHE:HZ    | 4:e:169:LEU:HD12  | 1.67                     | 0.59              |
| 9:j:35:ARG:HA     | 9:j:40:HIS:CD2    | 2.38                     | 0.59              |
| 32:G:32:GLY:HA2   | 32:G:38:HIS:HA    | 1.84                     | 0.59              |
| 44:S:4:SER:OG     | 53:3:1216:A:H5''  | 2.02                     | 0.59              |
| 53:3:314:C:O2'    | 53:3:315:A:H5'    | 2.02                     | 0.59              |
| 53:3:1202:U:H2'   | 53:3:1203:C:C6    | 2.37                     | 0.59              |
| 59:8:62:THR:HG22  | 59:8:64:THR:H     | 1.67                     | 0.59              |
| 59:8:315:GLU:HG3  | 59:8:316:PRO:HD2  | 1.84                     | 0.59              |
| 5:f:102:ILE:HD11  | 5:f:147:LEU:HD21  | 1.85                     | 0.59              |
| 10:k:42:THR:C     | 10:k:43:ILE:HD12  | 2.28                     | 0.59              |
| 19:t:29:THR:CG2   | 19:t:86:THR:HG22  | 2.33                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:A:62:LYS:NZ   | 49:X:17:LYS:HD3   | 2.17                     | 0.59              |
| 40:O:18:ILE:HG23 | 40:O:72:ARG:NH1   | 2.17                     | 0.59              |
| 53:3:1299:A:H2'  | 53:3:1300:G:H4'   | 1.84                     | 0.59              |
| 54:1:193:U:O2'   | 54:1:194:G:H5'    | 2.03                     | 0.59              |
| 54:1:2156:G:H2'  | 54:1:2157:G:H5'   | 1.85                     | 0.59              |
| 58:4:8:A:H2'     | 58:4:9:G:H5'      | 1.84                     | 0.59              |
| 59:8:29:ARG:HA   | 59:8:29:ARG:HE    | 1.68                     | 0.59              |
| 8:i:56:VAL:HG21  | 8:i:68:PHE:CD2    | 2.38                     | 0.59              |
| 35:J:156:ARG:HA  | 35:J:158:LYS:HZ2  | 1.67                     | 0.59              |
| 43:R:98:GLY:N    | 53:3:1308:U:C6    | 2.70                     | 0.59              |
| 54:1:580:U:H2'   | 54:1:581:C:H6     | 1.65                     | 0.59              |
| 34:I:25:ARG:HH12 | 34:I:30:LYS:NZ    | 2.00                     | 0.59              |
| 40:O:17:LEU:O    | 40:O:20:GLN:HG3   | 2.02                     | 0.59              |
| 49:X:52:ASN:HD21 | 49:X:55:GLN:HG3   | 1.67                     | 0.59              |
| 53:3:919:A:H2    | 53:3:1080:A:H62   | 1.46                     | 0.59              |
| 53:3:1122:U:H2'  | 53:3:1123:U:C6    | 2.38                     | 0.59              |
| 54:1:880:G:H2'   | 54:1:881:G:H8     | 1.67                     | 0.59              |
| 54:1:1060:U:H4'  | 54:1:1061:U:C5'   | 2.33                     | 0.59              |
| 54:1:1545:A:H2'  | 54:1:1546:G:O4'   | 2.03                     | 0.59              |
| 54:1:1725:U:H2'  | 54:1:1726:C:C6    | 2.38                     | 0.59              |
| 54:1:1917:U:O2'  | 54:1:1918:A:H5'   | 2.02                     | 0.59              |
| 2:c:122:VAL:HG11 | 2:c:141:ARG:HH12  | 1.68                     | 0.59              |
| 6:g:85:GLY:N     | 6:g:89:LYS:O      | 2.26                     | 0.59              |
| 6:g:116:ARG:O    | 6:g:118:PRO:HD3   | 2.03                     | 0.59              |
| 9:j:30:THR:HG21  | 54:1:1005:C:O2'   | 2.03                     | 0.59              |
| 11:l:115:GLU:H   | 11:l:115:GLU:CD   | 2.11                     | 0.59              |
| 22:w:19:VAL:HG12 | 22:w:21:ARG:O     | 2.02                     | 0.59              |
| 34:I:104:MET:HE1 | 34:I:172:VAL:HA   | 1.84                     | 0.59              |
| 37:L:78:ARG:HG2  | 37:L:82:SER:O     | 2.02                     | 0.59              |
| 40:O:40:ILE:CG1  | 40:O:73:LEU:HD12  | 2.32                     | 0.59              |
| 47:V:5:ARG:HD3   | 53:3:636:U:H5''   | 1.85                     | 0.59              |
| 54:1:741:U:H2'   | 54:1:742:A:C8     | 2.38                     | 0.59              |
| 54:1:2329:U:H2'  | 54:1:2330:G:C8    | 2.38                     | 0.59              |
| 55:2:119:A:N3    | 55:2:120:A:C1'    | 2.65                     | 0.59              |
| 59:8:18:HIS:HB2  | 59:8:123:SER:HB2  | 1.83                     | 0.59              |
| 59:8:61:ILE:HB   | 59:8:92:HIS:HE1   | 1.68                     | 0.59              |
| 59:8:121:PRO:C   | 59:8:123:SER:N    | 2.40                     | 0.59              |
| 59:8:362:ARG:O   | 59:8:386:ILE:HG22 | 2.03                     | 0.59              |
| 3:d:29:HIS:CD2   | 11:l:8:PRO:HA     | 2.37                     | 0.59              |
| 7:h:22:ALA:C     | 7:h:23:LEU:HD12   | 2.28                     | 0.59              |
| 11:l:33:ARG:HH12 | 54:1:671:C:P      | 2.25                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:l:38:GLN:HG3  | 54:l:805:G:O4'    | 2.03                     | 0.59              |
| 16:q:111:LYS:HG2 | 17:r:48:LYS:NZ    | 2.17                     | 0.59              |
| 34:I:56:GLU:HG3  | 34:I:198:LEU:HD12 | 1.84                     | 0.59              |
| 37:L:119:LEU:O   | 37:L:123:LEU:HG   | 2.03                     | 0.59              |
| 40:O:40:ILE:O    | 53:3:1123:U:O2    | 2.21                     | 0.59              |
| 49:X:47:THR:HG22 | 49:X:60:PHE:HA    | 1.85                     | 0.59              |
| 54:1:1373:A:H5'  | 54:1:2212:A:H1'   | 1.84                     | 0.59              |
| 54:1:2111:U:H5'  | 54:1:2112:G:OP2   | 2.02                     | 0.59              |
| 54:1:2670:A:H2'  | 54:1:2671:G:H8    | 1.68                     | 0.59              |
| 57:6:13:C:H2'    | 57:6:14:A:H5''    | 1.85                     | 0.59              |
| 59:8:411:PHE:N   | 59:8:412:PRO:HD3  | 2.18                     | 0.59              |
| 3:d:40:ARG:HG2   | 3:d:40:ARG:HH11   | 1.68                     | 0.58              |
| 4:e:12:VAL:O     | 4:e:16:MET:HG2    | 2.03                     | 0.58              |
| 4:e:140:ILE:N    | 4:e:140:ILE:HD12  | 2.18                     | 0.58              |
| 31:F:32:LYS:HE3  | 54:1:2478:A:H5'   | 1.85                     | 0.58              |
| 32:G:46:VAL:HB   | 32:G:47:PRO:HD3   | 1.83                     | 0.58              |
| 33:H:87:ARG:HB3  | 33:H:87:ARG:HH11  | 1.66                     | 0.58              |
| 39:N:89:TYR:CB   | 39:N:93:LEU:HD12  | 2.32                     | 0.58              |
| 41:P:19:VAL:HG12 | 41:P:82:GLU:HG3   | 1.84                     | 0.58              |
| 42:Q:35:ARG:HB3  | 42:Q:53:ARG:HB3   | 1.85                     | 0.58              |
| 43:R:48:SER:HB3  | 43:R:51:GLN:OE1   | 2.03                     | 0.58              |
| 47:V:29:LYS:HB2  | 47:V:36:PHE:CZ    | 2.38                     | 0.58              |
| 53:3:1317:C:H5'  | 53:3:1318:A:OP2   | 2.03                     | 0.58              |
| 53:3:1343:G:H2'  | 53:3:1344:C:C6    | 2.37                     | 0.58              |
| 54:1:1054:A:H2'  | 54:1:1055:G:O4'   | 2.03                     | 0.58              |
| 1:b:95:TYR:HE2   | 1:b:101:ARG:HD2   | 1.67                     | 0.58              |
| 6:g:39:ALA:HA    | 6:g:43:ASN:HB2    | 1.85                     | 0.58              |
| 6:g:112:LYS:HA   | 6:g:115:VAL:HB    | 1.85                     | 0.58              |
| 8:i:25:PRO:HB3   | 8:i:29:GLN:HG2    | 1.84                     | 0.58              |
| 15:p:102:ARG:HG2 | 15:p:102:ARG:HH11 | 1.68                     | 0.58              |
| 21:v:42:LEU:HD13 | 21:v:47:VAL:HG21  | 1.85                     | 0.58              |
| 24:y:23:ARG:H    | 24:y:23:ARG:HD3   | 1.68                     | 0.58              |
| 31:F:36:ARG:HD2  | 31:F:37:GLN:N     | 2.17                     | 0.58              |
| 32:G:175:ALA:HB1 | 32:G:180:ILE:HB   | 1.84                     | 0.58              |
| 34:I:74:TYR:CD1  | 34:I:92:LEU:HD23  | 2.38                     | 0.58              |
| 40:O:38:GLY:O    | 53:3:1124:G:OP1   | 2.20                     | 0.58              |
| 53:3:1080:A:OP2  | 53:3:1081:A:H5'   | 2.04                     | 0.58              |
| 54:1:17:G:H2'    | 54:1:18:U:C6      | 2.38                     | 0.58              |
| 54:1:1912:A:H62  | 54:1:1917:U:H3    | 1.51                     | 0.58              |
| 59:8:424:THR:O   | 59:8:427:ASP:N    | 2.32                     | 0.58              |
| 2:c:13:ARG:HG2   | 15:p:55:HIS:CE1   | 2.38                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:t:64:LYS:HE2   | 19:t:64:LYS:CA    | 2.33                     | 0.58              |
| 35:J:28:ARG:HD2   | 35:J:28:ARG:N     | 2.18                     | 0.58              |
| 36:K:49:TYR:CE1   | 48:W:65:SER:HA    | 2.38                     | 0.58              |
| 49:X:9:PHE:CE1    | 53:3:1318:A:H4'   | 2.39                     | 0.58              |
| 52:a:23:ILE:HD12  | 52:a:23:ILE:N     | 2.18                     | 0.58              |
| 54:1:1170:C:H2'   | 54:1:1171:G:C8    | 2.38                     | 0.58              |
| 59:8:63:ILE:HD12  | 59:8:63:ILE:N     | 2.17                     | 0.58              |
| 59:8:620:GLU:O    | 59:8:680:TYR:HB2  | 2.04                     | 0.58              |
| 6:g:9:VAL:HG12    | 6:g:13:GLY:HA3    | 1.85                     | 0.58              |
| 14:o:43:ASN:ND2   | 14:o:45:SER:HB3   | 2.18                     | 0.58              |
| 22:w:17:LEU:HD11  | 22:w:37:ARG:HH21  | 1.68                     | 0.58              |
| 22:w:17:LEU:HD21  | 22:w:37:ARG:NE    | 2.18                     | 0.58              |
| 34:I:124:VAL:HG22 | 34:I:125:ASN:ND2  | 2.18                     | 0.58              |
| 37:L:99:ALA:HA    | 37:L:102:TRP:CE3  | 2.39                     | 0.58              |
| 44:S:48:GLN:HE21  | 49:X:9:PHE:HE1    | 1.49                     | 0.58              |
| 53:3:300:A:H2'    | 53:3:301:G:O4'    | 2.03                     | 0.58              |
| 54:1:1319:C:O2'   | 54:1:1320:C:H5'   | 2.04                     | 0.58              |
| 54:1:2569:G:O2'   | 54:1:2570:G:H5'   | 2.03                     | 0.58              |
| 59:8:514:GLN:HB3  | 59:8:592:ALA:HB2  | 1.84                     | 0.58              |
| 1:b:44:ASN:ND2    | 54:1:1812:U:H1'   | 2.19                     | 0.58              |
| 2:c:146:ILE:HD11  | 2:c:155:VAL:HG11  | 1.85                     | 0.58              |
| 5:f:93:TYR:HA     | 5:f:105:SER:O     | 2.03                     | 0.58              |
| 9:j:17:VAL:HA     | 9:j:55:ILE:HG22   | 1.84                     | 0.58              |
| 35:J:10:LEU:HD12  | 35:J:11:GLN:H     | 1.68                     | 0.58              |
| 38:M:9:MET:HG2    | 38:M:26:MET:HE1   | 1.85                     | 0.58              |
| 42:Q:112:ALA:HB1  | 42:Q:115:LYS:NZ   | 2.17                     | 0.58              |
| 52:a:48:LEU:CD2   | 52:a:209:ILE:HG12 | 2.34                     | 0.58              |
| 53:3:33:A:H2'     | 53:3:34:C:H6      | 1.63                     | 0.58              |
| 53:3:1288:A:O2'   | 53:3:1353:G:H5'   | 2.04                     | 0.58              |
| 53:3:1406:U:H2'   | 53:3:1407:C:H6    | 1.67                     | 0.58              |
| 54:1:818:G:O2'    | 54:1:819:A:H5''   | 2.03                     | 0.58              |
| 54:1:1549:A:H2'   | 54:1:1550:C:C6    | 2.38                     | 0.58              |
| 54:1:2098:U:H2'   | 54:1:2099:U:O4'   | 2.04                     | 0.58              |
| 59:8:142:ASN:CG   | 59:8:143:LYS:H    | 2.11                     | 0.58              |
| 37:L:125:ASP:HB2  | 37:L:131:GLY:N    | 2.19                     | 0.58              |
| 38:M:48:PHE:HB2   | 38:M:59:GLU:O     | 2.04                     | 0.58              |
| 40:O:56:HIS:HE1   | 53:3:963:G:H21    | 1.50                     | 0.58              |
| 53:3:408:A:H2'    | 53:3:409:U:O4'    | 2.04                     | 0.58              |
| 53:3:1171:A:C6    | 53:3:1172:C:C2    | 2.90                     | 0.58              |
| 54:1:2122:U:H2'   | 54:1:2123:G:C8    | 2.38                     | 0.58              |
| 54:1:2716:C:O2'   | 54:1:2717:C:H5'   | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 59:8:16:SER:HA    | 59:8:90:PRO:HG3   | 1.86                     | 0.58              |
| 59:8:561:LEU:HD23 | 59:8:561:LEU:O    | 2.04                     | 0.58              |
| 4:e:3:LEU:CA      | 4:e:6:TYR:HB3     | 2.30                     | 0.58              |
| 5:f:163:TYR:HB2   | 5:f:166:GLU:CG    | 2.34                     | 0.58              |
| 20:u:65:GLN:HB2   | 20:u:68:ASN:HB2   | 1.86                     | 0.58              |
| 32:G:19:THR:HG23  | 32:G:21:TYR:O     | 2.02                     | 0.58              |
| 36:K:7:VAL:HG13   | 36:K:60:VAL:O     | 2.03                     | 0.58              |
| 40:O:36:VAL:HG11  | 53:3:1123:U:OP1   | 2.04                     | 0.58              |
| 41:P:118:ASN:OD1  | 53:3:717:U:H4'    | 2.04                     | 0.58              |
| 43:R:104:ASN:O    | 43:R:106:ARG:N    | 2.36                     | 0.58              |
| 44:S:15:LEU:CD1   | 44:S:53:ASP:HB2   | 2.34                     | 0.58              |
| 53:3:624:C:H2'    | 53:3:625:U:O4'    | 2.04                     | 0.58              |
| 54:1:1079:C:H2'   | 54:1:1080:A:C8    | 2.39                     | 0.58              |
| 57:6:46:G:C3'     | 57:6:47:U:H5'     | 2.32                     | 0.58              |
| 59:8:350:LEU:HD12 | 59:8:356:ALA:O    | 2.04                     | 0.58              |
| 59:8:598:SER:O    | 59:8:601:PHE:HB3  | 2.04                     | 0.58              |
| 14:o:30:ARG:HD2   | 14:o:102:ARG:NH1  | 2.18                     | 0.58              |
| 15:p:30:TRP:HZ3   | 15:p:39:LEU:HB2   | 1.69                     | 0.58              |
| 34:I:195:ASN:ND2  | 34:I:197:HIS:HB3  | 2.16                     | 0.58              |
| 35:J:64:GLU:CD    | 35:J:64:GLU:H     | 2.11                     | 0.58              |
| 45:T:80:LEU:HA    | 45:T:83:ARG:HD3   | 1.85                     | 0.58              |
| 53:3:477:C:H2'    | 53:3:478:A:C8     | 2.39                     | 0.58              |
| 53:3:585:G:H2'    | 53:3:586:C:C6     | 2.39                     | 0.58              |
| 53:3:676:A:H2'    | 53:3:677:U:C6     | 2.38                     | 0.58              |
| 53:3:856:C:O2'    | 53:3:857:C:H5'    | 2.04                     | 0.58              |
| 53:3:1062:U:H2'   | 53:3:1063:C:C4    | 2.39                     | 0.58              |
| 53:3:1115:U:C2'   | 53:3:1116:U:H5''  | 2.18                     | 0.58              |
| 54:1:1353:A:H2'   | 54:1:1354:A:C8    | 2.39                     | 0.58              |
| 54:1:1361:G:H2'   | 54:1:1362:C:C6    | 2.38                     | 0.58              |
| 54:1:2895:G:H2'   | 54:1:2896:C:C6    | 2.38                     | 0.58              |
| 59:8:19:ILE:HD13  | 59:8:92:HIS:NE2   | 2.18                     | 0.58              |
| 59:8:624:PRO:O    | 59:8:651:GLY:HA2  | 2.04                     | 0.58              |
| 7:h:54:VAL:HG12   | 54:1:1083:U:O3'   | 2.04                     | 0.58              |
| 14:o:73:ALA:HA    | 14:o:76:LYS:HE3   | 1.86                     | 0.58              |
| 24:y:20:ASN:O     | 24:y:24:GLU:HB2   | 2.04                     | 0.58              |
| 33:H:50:SER:HB2   | 33:H:71:ARG:NE    | 2.19                     | 0.58              |
| 33:H:188:ALA:O    | 33:H:194:VAL:HA   | 2.04                     | 0.58              |
| 34:I:108:ALA:HA   | 34:I:160:LEU:HD23 | 1.85                     | 0.58              |
| 43:R:78:ARG:HH12  | 49:X:68:HIS:CE1   | 2.22                     | 0.58              |
| 47:V:58:VAL:HG13  | 47:V:74:LEU:HD13  | 1.85                     | 0.58              |
| 52:a:208:TYR:CD2  | 52:a:209:ILE:HG13 | 2.39                     | 0.58              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 54:1:1133:A:H4'   | 54:1:1134:A:H5'' | 1.86                     | 0.58              |
| 59:8:539:ASP:HB3  | 59:8:579:HIS:HA  | 1.85                     | 0.58              |
| 2:c:8:LYS:HB2     | 2:c:201:LEU:HD11 | 1.86                     | 0.58              |
| 28:C:4:ILE:HD12   | 28:C:4:ILE:N     | 2.18                     | 0.58              |
| 41:P:110:THR:HG23 | 51:Z:4:LYS:HB2   | 1.86                     | 0.58              |
| 42:Q:81:ILE:HD11  | 42:Q:96:THR:HG22 | 1.85                     | 0.58              |
| 42:Q:93:ARG:HG3   | 42:Q:93:ARG:HH11 | 1.69                     | 0.58              |
| 47:V:58:VAL:HG12  | 47:V:60:ILE:HG23 | 1.86                     | 0.58              |
| 53:3:15:G:C8      | 53:3:1396:A:O2'  | 2.57                     | 0.58              |
| 53:3:1202:U:H2'   | 53:3:1203:C:H6   | 1.68                     | 0.58              |
| 54:1:1138:G:H2'   | 54:1:1139:G:O4'  | 2.03                     | 0.58              |
| 54:1:1308:A:H2'   | 54:1:1309:G:H5'  | 1.85                     | 0.58              |
| 59:8:438:LEU:O    | 59:8:441:GLU:HG3 | 2.03                     | 0.58              |
| 5:f:49:LEU:CD1    | 5:f:71:LEU:HD21  | 2.32                     | 0.57              |
| 7:h:67:THR:N      | 7:h:68:PRO:HD3   | 2.18                     | 0.57              |
| 11:l:26:GLY:O     | 11:l:27:LEU:HD23 | 2.04                     | 0.57              |
| 15:p:108:ARG:HH12 | 53:3:1464:U:P    | 2.26                     | 0.57              |
| 16:q:111:LYS:HE2  | 17:r:48:LYS:NZ   | 2.18                     | 0.57              |
| 28:C:5:ARG:HG2    | 28:C:23:THR:OG1  | 2.04                     | 0.57              |
| 36:K:19:PRO:O     | 36:K:23:GLU:HG3  | 2.03                     | 0.57              |
| 40:O:53:ILE:HD12  | 44:S:84:ARG:CD   | 2.33                     | 0.57              |
| 42:Q:23:LEU:HD11  | 42:Q:58:ASN:HB3  | 1.86                     | 0.57              |
| 43:R:97:ARG:HG3   | 53:3:1308:U:C2   | 2.39                     | 0.57              |
| 44:S:5:MET:CG     | 44:S:62:ARG:HH22 | 2.16                     | 0.57              |
| 49:X:47:THR:HG22  | 49:X:60:PHE:HB2  | 1.86                     | 0.57              |
| 49:X:59:VAL:HG11  | 49:X:73:PHE:HB2  | 1.86                     | 0.57              |
| 53:3:41:G:H2'     | 53:3:42:G:H8     | 1.69                     | 0.57              |
| 54:1:566:U:H4'    | 54:1:809:G:P     | 2.44                     | 0.57              |
| 59:8:268:SER:HB3  | 59:8:271:LYS:HB2 | 1.85                     | 0.57              |
| 59:8:299:LEU:HD11 | 59:8:403:PRO:HD2 | 1.85                     | 0.57              |
| 4:e:139:GLU:HG3   | 26:A:28:VAL:HG22 | 1.85                     | 0.57              |
| 8:i:25:PRO:HD3    | 59:8:646:GLU:HA  | 1.84                     | 0.57              |
| 10:k:13:ASN:HD21  | 10:k:98:ARG:N    | 2.02                     | 0.57              |
| 19:t:13:ALA:HB3   | 19:t:33:LYS:HD3  | 1.86                     | 0.57              |
| 32:G:132:GLU:HA   | 32:G:135:MET:CE  | 2.33                     | 0.57              |
| 35:J:111:ARG:HH11 | 35:J:111:ARG:HG3 | 1.68                     | 0.57              |
| 38:M:12:ARG:HD2   | 38:M:26:MET:SD   | 2.44                     | 0.57              |
| 45:T:50:HIS:CE1   | 53:3:667:G:H4'   | 2.39                     | 0.57              |
| 46:U:5:ARG:H      | 46:U:5:ARG:HD3   | 1.69                     | 0.57              |
| 53:3:924:C:H4'    | 53:3:1399:C:H5'' | 1.86                     | 0.57              |
| 53:3:1167:A:C2    | 53:3:1169:A:C8   | 2.92                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:1103:A:H3'   | 54:1:1104:C:C6    | 2.39                     | 0.57              |
| 7:h:41:LEU:HD13   | 54:1:1083:U:O5'   | 2.03                     | 0.57              |
| 17:r:68:ARG:NH1   | 17:r:90:ARG:HB2   | 2.20                     | 0.57              |
| 23:x:16:ASN:OD1   | 23:x:26:ARG:HD2   | 2.03                     | 0.57              |
| 34:I:145:ARG:CZ   | 34:I:147:LYS:HE3  | 2.35                     | 0.57              |
| 35:J:29:ILE:HG23  | 35:J:53:ARG:HH12  | 1.68                     | 0.57              |
| 35:J:156:ARG:NH2  | 38:M:42:GLU:HG3   | 2.19                     | 0.57              |
| 38:M:9:MET:SD     | 38:M:13:ILE:HD11  | 2.44                     | 0.57              |
| 38:M:12:ARG:NH2   | 53:3:826:C:H5'    | 2.19                     | 0.57              |
| 40:O:38:GLY:O     | 53:3:1124:G:P     | 2.62                     | 0.57              |
| 41:P:34:THR:HB    | 41:P:40:ALA:HA    | 1.86                     | 0.57              |
| 51:Z:32:ARG:NH1   | 51:Z:33:ARG:HG3   | 2.16                     | 0.57              |
| 53:3:350:G:H2'    | 53:3:351:G:C8     | 2.38                     | 0.57              |
| 53:3:1033:G:C2'   | 53:3:1034:G:H5''  | 2.29                     | 0.57              |
| 53:3:1436:U:H2'   | 53:3:1437:A:H8    | 1.69                     | 0.57              |
| 54:1:1401:G:H2'   | 54:1:1402:U:C6    | 2.39                     | 0.57              |
| 54:1:2515:C:H2'   | 54:1:2516:A:C8    | 2.39                     | 0.57              |
| 55:2:88:C:H5''    | 55:2:89:U:OP1     | 2.04                     | 0.57              |
| 6:g:129:GLU:HG2   | 6:g:143:ILE:HG12  | 1.86                     | 0.57              |
| 40:O:39:PRO:HB3   | 53:3:1123:U:C4    | 2.39                     | 0.57              |
| 41:P:126:ARG:HB3  | 51:Z:33:ARG:HH12  | 1.68                     | 0.57              |
| 43:R:97:ARG:CB    | 53:3:1307:U:C2    | 2.83                     | 0.57              |
| 51:Z:32:ARG:HH11  | 51:Z:33:ARG:CG    | 2.15                     | 0.57              |
| 53:3:271:C:H2'    | 53:3:272:C:C6     | 2.38                     | 0.57              |
| 53:3:1211:U:H4'   | 53:3:1213:A:C4    | 2.40                     | 0.57              |
| 53:3:1435:G:H2'   | 53:3:1436:U:H6    | 1.66                     | 0.57              |
| 54:1:1874:C:H2'   | 54:1:1875:G:O4'   | 2.04                     | 0.57              |
| 54:1:2543:G:H2'   | 54:1:2544:G:H8    | 1.68                     | 0.57              |
| 59:8:359:ARG:HG2  | 59:8:360:PHE:N    | 2.17                     | 0.57              |
| 7:h:43:LYS:HA     | 7:h:46:ARG:NH1    | 2.19                     | 0.57              |
| 15:p:83:ILE:HD12  | 15:p:83:ILE:N     | 2.20                     | 0.57              |
| 53:3:407:U:H2'    | 53:3:408:A:C8     | 2.39                     | 0.57              |
| 14:o:87:ILE:HD12  | 14:o:87:ILE:N     | 2.18                     | 0.57              |
| 40:O:53:ILE:HG21  | 53:3:1061:G:OP1   | 2.04                     | 0.57              |
| 52:a:23:ILE:H     | 52:a:23:ILE:CD1   | 2.16                     | 0.57              |
| 53:3:893:C:H2'    | 53:3:894:G:C8     | 2.40                     | 0.57              |
| 59:8:169:LEU:HD22 | 59:8:263:LEU:HD22 | 1.87                     | 0.57              |
| 5:f:26:LYS:HB2    | 5:f:31:GLU:OE2    | 2.04                     | 0.57              |
| 9:j:40:HIS:CE1    | 9:j:41:LYS:HG3    | 2.40                     | 0.57              |
| 17:r:48:LYS:HD2   | 17:r:49:ILE:O     | 2.05                     | 0.57              |
| 20:u:46:LYS:HG2   | 20:u:47:PRO:HD2   | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:w:37:ARG:HD2   | 54:1:2387:U:H1'   | 1.87                     | 0.57              |
| 44:S:35:ALA:HB1   | 44:S:39:ASP:HB3   | 1.86                     | 0.57              |
| 46:U:33:ILE:N     | 46:U:33:ILE:HD12  | 2.20                     | 0.57              |
| 53:3:1075:U:H2'   | 53:3:1076:U:C6    | 2.39                     | 0.57              |
| 53:3:1327:C:O2'   | 53:3:1328:C:H5'   | 2.04                     | 0.57              |
| 54:1:1019:U:H3    | 54:1:1142:A:H62   | 1.51                     | 0.57              |
| 54:1:1086:A:H1'   | 54:1:1103:A:N1    | 2.20                     | 0.57              |
| 54:1:2457:U:H3    | 54:1:2494:G:H1    | 1.50                     | 0.57              |
| 4:e:32:LYS:NZ     | 54:1:2314:A:H5''  | 2.19                     | 0.57              |
| 9:j:47:HIS:ND1    | 9:j:48:VAL:HG13   | 2.20                     | 0.57              |
| 11:l:30:THR:HG22  | 54:1:810:U:O4     | 2.04                     | 0.57              |
| 13:n:30:ARG:NH1   | 13:n:75:ILE:HD11  | 2.19                     | 0.57              |
| 22:w:25:GLU:HG3   | 54:1:923:G:H4'    | 1.87                     | 0.57              |
| 26:A:64:PHE:CE1   | 53:3:1011:C:H4'   | 2.39                     | 0.57              |
| 36:K:11:HIS:ND1   | 36:K:54:LEU:HD13  | 2.18                     | 0.57              |
| 45:T:2:LEU:HD21   | 45:T:33:ALA:HB3   | 1.87                     | 0.57              |
| 45:T:55:LEU:O     | 45:T:59:VAL:HG23  | 2.05                     | 0.57              |
| 46:U:19:VAL:HG13  | 46:U:36:VAL:O     | 2.05                     | 0.57              |
| 52:a:170:ILE:HD13 | 54:1:2177:C:O2    | 2.04                     | 0.57              |
| 52:a:200:LYS:HZ3  | 52:a:208:TYR:HB2  | 1.70                     | 0.57              |
| 53:3:1049:U:H4'   | 53:3:1050:G:H5''  | 1.87                     | 0.57              |
| 54:1:891:G:H2'    | 54:1:892:A:H8     | 1.69                     | 0.57              |
| 54:1:2131:U:O5'   | 54:1:2133:G:H4'   | 2.05                     | 0.57              |
| 56:5:16:C:O2      | 56:5:60:U:H4'     | 2.05                     | 0.57              |
| 1:b:35:LYS:HG2    | 1:b:36:ASN:N      | 2.20                     | 0.57              |
| 8:i:25:PRO:HD2    | 59:8:645:GLN:HE22 | 1.69                     | 0.57              |
| 9:j:101:ILE:HD12  | 9:j:101:ILE:N     | 2.20                     | 0.57              |
| 15:p:113:LEU:O    | 15:p:113:LEU:HD12 | 2.05                     | 0.57              |
| 26:A:59:ARG:CZ    | 49:X:17:LYS:HZ3   | 2.18                     | 0.57              |
| 46:U:5:ARG:CG     | 53:3:376:G:H5''   | 2.34                     | 0.57              |
| 46:U:20:VAL:HG22  | 46:U:21:VAL:N     | 2.20                     | 0.57              |
| 47:V:37:ILE:HG13  | 47:V:38:LYS:N     | 2.20                     | 0.57              |
| 50:Y:11:ILE:HG13  | 50:Y:12:GLN:N     | 2.19                     | 0.57              |
| 53:3:16:A:C2      | 53:3:17:U:C6      | 2.92                     | 0.57              |
| 53:3:256:U:H2'    | 53:3:257:G:C8     | 2.39                     | 0.57              |
| 54:1:310:A:O2'    | 54:1:311:A:H5''   | 2.05                     | 0.57              |
| 54:1:1565:C:O2'   | 54:1:1566:A:H2'   | 2.05                     | 0.57              |
| 54:1:2670:A:H2'   | 54:1:2671:G:C8    | 2.40                     | 0.57              |
| 59:8:152:LEU:O    | 59:8:155:VAL:HG22 | 2.05                     | 0.57              |
| 59:8:299:LEU:N    | 59:8:304:ASP:O    | 2.37                     | 0.57              |
| 1:b:54:GLY:HA3    | 1:b:216:ARG:CD    | 2.34                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:b:152:GLN:HB3  | 54:1:1818:U:N3    | 2.19                     | 0.57              |
| 4:e:32:LYS:HB3   | 4:e:91:ARG:HG3    | 1.87                     | 0.57              |
| 40:O:14:ASP:OD1  | 40:O:16:ARG:HG2   | 2.05                     | 0.57              |
| 42:Q:43:LYS:HB2  | 53:3:1492:A:OP1   | 2.05                     | 0.57              |
| 53:3:76:G:H1     | 53:3:93:U:H3      | 1.53                     | 0.57              |
| 53:3:179:A:H61   | 53:3:196:A:H62    | 1.52                     | 0.57              |
| 53:3:270:A:H2'   | 53:3:271:C:C6     | 2.40                     | 0.57              |
| 54:1:1400:U:H2'  | 54:1:1401:G:C8    | 2.40                     | 0.57              |
| 59:8:100:GLU:OE2 | 59:8:412:PRO:HG3  | 2.03                     | 0.57              |
| 4:e:65:LEU:HD13  | 55:2:42:C:C6      | 2.40                     | 0.56              |
| 5:f:9:VAL:HA     | 5:f:48:THR:CG2    | 2.34                     | 0.56              |
| 5:f:174:LYS:HG2  | 54:1:2529:G:H5'   | 1.88                     | 0.56              |
| 19:t:59:ASN:HB3  | 54:1:1341:G:H1'   | 1.87                     | 0.56              |
| 20:u:4:ILE:HD12  | 20:u:4:ILE:N      | 2.20                     | 0.56              |
| 23:x:36:ARG:HA   | 23:x:47:THR:HA    | 1.86                     | 0.56              |
| 49:X:36:ARG:HG2  | 53:3:1320:C:C5    | 2.40                     | 0.56              |
| 53:3:16:A:C2     | 53:3:1080:A:C4    | 2.93                     | 0.56              |
| 53:3:89:U:H2'    | 53:3:90:C:O4'     | 2.05                     | 0.56              |
| 53:3:1356:G:H2'  | 53:3:1357:A:C8    | 2.39                     | 0.56              |
| 54:1:222:A:N6    | 54:1:232:G:H1'    | 2.19                     | 0.56              |
| 59:8:23:LYS:HE3  | 59:8:90:PRO:CG    | 2.35                     | 0.56              |
| 59:8:54:GLU:HG3  | 59:8:55:GLN:NE2   | 2.19                     | 0.56              |
| 17:r:6:GLN:HG2   | 17:r:11:GLN:NE2   | 2.20                     | 0.56              |
| 18:s:98:LYS:HD3  | 54:1:2012:G:OP1   | 2.04                     | 0.56              |
| 39:N:95:SER:O    | 39:N:99:LYS:HD3   | 2.05                     | 0.56              |
| 40:O:8:ILE:HG13  | 40:O:100:ILE:HG22 | 1.86                     | 0.56              |
| 40:O:52:LEU:HB2  | 44:S:80:ARG:CD    | 2.33                     | 0.56              |
| 53:3:530:G:H3'   | 53:3:531:U:C5'    | 2.35                     | 0.56              |
| 53:3:853:C:H2'   | 53:3:854:U:C6     | 2.40                     | 0.56              |
| 53:3:927:G:O2'   | 53:3:1532:U:H4'   | 2.04                     | 0.56              |
| 53:3:1079:G:C2'  | 53:3:1080:A:H5'   | 2.35                     | 0.56              |
| 53:3:1370:G:H2'  | 53:3:1371:G:H8    | 1.69                     | 0.56              |
| 54:1:281:C:N4    | 54:1:359:G:H1     | 2.03                     | 0.56              |
| 54:1:414:C:H2'   | 54:1:415:A:C8     | 2.40                     | 0.56              |
| 54:1:1020:A:H1'  | 54:1:1021:A:OP2   | 2.04                     | 0.56              |
| 59:8:627:ASN:O   | 59:8:631:VAL:HG23 | 2.06                     | 0.56              |
| 5:f:68:ARG:HD3   | 5:f:68:ARG:C      | 2.30                     | 0.56              |
| 11:l:77:ILE:HD12 | 11:l:77:ILE:N     | 2.20                     | 0.56              |
| 17:r:68:ARG:HB2  | 17:r:90:ARG:HH21  | 1.69                     | 0.56              |
| 18:s:85:ILE:HG23 | 18:s:93:ALA:HB1   | 1.87                     | 0.56              |
| 21:v:6:ALA:HB3   | 21:v:63:ILE:HD11  | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:z:23:LEU:HD21  | 25:z:53:MET:CE    | 2.35                     | 0.56              |
| 31:F:36:ARG:CD    | 31:F:37:GLN:H     | 2.17                     | 0.56              |
| 33:H:152:VAL:HG13 | 33:H:197:VAL:HG22 | 1.87                     | 0.56              |
| 33:H:166:TRP:CH2  | 53:3:1192:C:H4'   | 2.40                     | 0.56              |
| 34:I:104:MET:HB3  | 34:I:106:PHE:CE2  | 2.39                     | 0.56              |
| 35:J:67:ARG:HB2   | 35:J:67:ARG:HH11  | 1.69                     | 0.56              |
| 35:J:132:PRO:HG2  | 35:J:133:ILE:HD12 | 1.87                     | 0.56              |
| 35:J:156:ARG:HA   | 35:J:158:LYS:NZ   | 2.20                     | 0.56              |
| 37:L:109:LYS:HG3  | 37:L:110:ARG:H    | 1.69                     | 0.56              |
| 44:S:92:ILE:N     | 44:S:92:ILE:HD12  | 2.21                     | 0.56              |
| 49:X:44:ILE:HD13  | 49:X:63:ASP:HA    | 1.88                     | 0.56              |
| 52:a:47:ASN:HB3   | 52:a:211:LYS:HB2  | 1.88                     | 0.56              |
| 53:3:15:G:O6      | 53:3:1080:A:C2    | 2.58                     | 0.56              |
| 53:3:41:G:H2'     | 53:3:42:G:C8      | 2.40                     | 0.56              |
| 53:3:451:A:H4'    | 53:3:452:A:O5'    | 2.04                     | 0.56              |
| 53:3:945:G:H1'    | 53:3:1337:G:O2'   | 2.04                     | 0.56              |
| 53:3:949:A:H2'    | 53:3:950:U:C6     | 2.41                     | 0.56              |
| 54:1:340:A:H2'    | 54:1:341:C:O4'    | 2.06                     | 0.56              |
| 54:1:499:U:H2'    | 54:1:500:G:O4'    | 2.05                     | 0.56              |
| 54:1:666:A:H2'    | 54:1:667:U:C6     | 2.39                     | 0.56              |
| 54:1:1278:C:H2'   | 54:1:1279:G:H8    | 1.70                     | 0.56              |
| 54:1:1999:C:O2'   | 54:1:2000:C:H5'   | 2.05                     | 0.56              |
| 54:1:2176:A:H2'   | 54:1:2177:C:C6    | 2.40                     | 0.56              |
| 54:1:2233:U:H2'   | 54:1:2234:G:C8    | 2.41                     | 0.56              |
| 55:2:104:A:H2'    | 55:2:105:G:O4'    | 2.05                     | 0.56              |
| 59:8:94:ASP:CG    | 59:8:464:LEU:HB2  | 2.30                     | 0.56              |
| 7:h:26:VAL:HG12   | 7:h:82:ILE:HG23   | 1.87                     | 0.56              |
| 13:n:103:ARG:HE   | 13:n:110:MET:HE1  | 1.70                     | 0.56              |
| 26:A:13:THR:HB    | 26:A:31:ASP:HB2   | 1.86                     | 0.56              |
| 34:I:115:GLN:NE2  | 34:I:153:ARG:HH12 | 2.02                     | 0.56              |
| 34:I:171:GLU:HB3  | 34:I:180:THR:HB   | 1.88                     | 0.56              |
| 52:a:4:LEU:HA     | 52:a:8:MET:SD     | 2.45                     | 0.56              |
| 54:1:435:C:H2'    | 54:1:436:C:H5'    | 1.87                     | 0.56              |
| 54:1:622:G:H2'    | 54:1:623:C:H6     | 1.71                     | 0.56              |
| 54:1:758:C:O2     | 54:1:758:C:H2'    | 2.06                     | 0.56              |
| 54:1:2127:G:H2'   | 54:1:2128:G:O4'   | 2.06                     | 0.56              |
| 54:1:2186:G:H2'   | 54:1:2187:U:C6    | 2.40                     | 0.56              |
| 59:8:391:VAL:HG23 | 59:8:391:VAL:O    | 2.06                     | 0.56              |
| 59:8:414:PRO:HB2  | 59:8:459:ALA:HB1  | 1.87                     | 0.56              |
| 9:j:53:TYR:CE1    | 9:j:121:LYS:HD3   | 2.40                     | 0.56              |
| 32:G:35:ASN:HB3   | 32:G:37:VAL:CG1   | 2.35                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:N:30:ASN:OD1   | 39:N:65:THR:HA    | 2.05                     | 0.56              |
| 53:3:135:C:C2'    | 53:3:136:C:H5'    | 2.34                     | 0.56              |
| 53:3:552:U:O2'    | 53:3:553:A:H5'    | 2.06                     | 0.56              |
| 53:3:939:G:H2'    | 53:3:940:C:C6     | 2.40                     | 0.56              |
| 9:j:45:THR:HB     | 9:j:48:VAL:CG2    | 2.35                     | 0.56              |
| 32:G:66:ILE:N     | 32:G:66:ILE:HD12  | 2.20                     | 0.56              |
| 33:H:72:PRO:O     | 33:H:76:ILE:HG12  | 2.05                     | 0.56              |
| 40:O:15:HIS:O     | 40:O:18:ILE:HG22  | 2.04                     | 0.56              |
| 49:X:45:GLY:HA2   | 49:X:60:PHE:HE1   | 1.70                     | 0.56              |
| 53:3:32:A:H2'     | 53:3:33:A:C8      | 2.41                     | 0.56              |
| 53:3:361:G:H2'    | 53:3:362:G:O4'    | 2.05                     | 0.56              |
| 53:3:1129:C:H2'   | 53:3:1139:G:N7    | 2.20                     | 0.56              |
| 53:3:1414:U:H2'   | 53:3:1415:G:H8    | 1.71                     | 0.56              |
| 54:1:1053:C:C3'   | 54:1:1054:A:H5''  | 2.35                     | 0.56              |
| 54:1:1893:C:C2'   | 54:1:1894:C:H5'   | 2.36                     | 0.56              |
| 54:1:2543:G:H2'   | 54:1:2544:G:C8    | 2.41                     | 0.56              |
| 54:1:2849:U:H4'   | 54:1:2868:A:C2    | 2.41                     | 0.56              |
| 59:8:315:GLU:OE2  | 59:8:316:PRO:HD2  | 2.06                     | 0.56              |
| 4:e:101:ARG:HH21  | 4:e:101:ARG:HG3   | 1.70                     | 0.56              |
| 13:n:12:ARG:HB2   | 13:n:12:ARG:HH21  | 1.71                     | 0.56              |
| 22:w:17:LEU:HD12  | 22:w:17:LEU:N     | 2.20                     | 0.56              |
| 32:G:206:ILE:O    | 32:G:209:VAL:HG22 | 2.06                     | 0.56              |
| 33:H:11:LEU:HD22  | 33:H:17:TRP:CD1   | 2.40                     | 0.56              |
| 38:M:60:LEU:N     | 38:M:60:LEU:HD23  | 2.21                     | 0.56              |
| 44:S:4:SER:O      | 44:S:8:ARG:HG2    | 2.06                     | 0.56              |
| 45:T:44:GLU:O     | 45:T:45:HIS:HB2   | 2.04                     | 0.56              |
| 52:a:49:GLY:HA2   | 52:a:210:LYS:HZ3  | 1.70                     | 0.56              |
| 54:1:1656:C:H2'   | 54:1:1657:U:H6    | 1.71                     | 0.56              |
| 54:1:1856:U:H2'   | 54:1:1857:G:O4'   | 2.06                     | 0.56              |
| 27:B:3:GLN:HA     | 54:1:2615:U:C2    | 2.41                     | 0.56              |
| 33:H:74:ILE:H     | 33:H:74:ILE:HD12  | 1.71                     | 0.56              |
| 33:H:137:VAL:HG11 | 33:H:167:TYR:CD2  | 2.41                     | 0.56              |
| 34:I:9:LYS:HA     | 34:I:12:ARG:NH1   | 2.20                     | 0.56              |
| 34:I:47:LEU:HD12  | 34:I:51:GLY:HA3   | 1.87                     | 0.56              |
| 35:J:56:PRO:O     | 35:J:59:ILE:HG12  | 2.06                     | 0.56              |
| 35:J:105:ILE:HG13 | 35:J:123:LEU:HA   | 1.88                     | 0.56              |
| 35:J:133:ILE:HD12 | 35:J:133:ILE:N    | 2.18                     | 0.56              |
| 38:M:79:ARG:HB2   | 38:M:80:PRO:HD2   | 1.87                     | 0.56              |
| 42:Q:85:ARG:HH21  | 42:Q:87:LYS:HA    | 1.70                     | 0.56              |
| 44:S:35:ALA:O     | 44:S:40:ARG:HG3   | 2.05                     | 0.56              |
| 47:V:24:ILE:HD12  | 47:V:24:ILE:N     | 2.21                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 47:V:32:ILE:HD12 | 47:V:32:ILE:N    | 2.20                     | 0.56              |
| 53:3:193:C:H2'   | 53:3:194:C:H6    | 1.70                     | 0.56              |
| 53:3:946:A:N6    | 53:3:1235:U:H3   | 2.01                     | 0.56              |
| 53:3:1054:C:C4   | 56:5:34:U:H1'    | 2.41                     | 0.56              |
| 53:3:1116:U:H1'  | 53:3:1185:G:C2   | 2.38                     | 0.56              |
| 53:3:1304:G:H2'  | 53:3:1305:G:H1'  | 1.86                     | 0.56              |
| 54:1:2031:A:C2   | 54:1:2498:C:H1'  | 2.41                     | 0.56              |
| 54:1:2179:C:H2'  | 54:1:2180:U:C6   | 2.40                     | 0.56              |
| 54:1:2537:U:H2'  | 54:1:2538:C:H6   | 1.69                     | 0.56              |
| 55:2:119:A:H2    | 55:2:120:A:H1'   | 1.70                     | 0.56              |
| 59:8:492:GLU:HG3 | 59:8:564:GLY:HA3 | 1.88                     | 0.56              |
| 1:b:107:LYS:HB2  | 1:b:193:GLU:HB3  | 1.88                     | 0.56              |
| 6:g:5:LEU:HD12   | 6:g:17:ASP:HB2   | 1.88                     | 0.56              |
| 7:h:34:THR:O     | 7:h:37:LYS:HE2   | 2.06                     | 0.56              |
| 32:G:76:SER:O    | 32:G:79:VAL:HG12 | 2.06                     | 0.56              |
| 40:O:57:VAL:CG2  | 40:O:58:ASN:H    | 2.15                     | 0.56              |
| 52:a:22:ASP:O    | 52:a:26:ALA:N    | 2.38                     | 0.56              |
| 53:3:919:A:H2'   | 53:3:920:U:O5'   | 2.06                     | 0.56              |
| 53:3:1233:G:H2'  | 53:3:1234:C:C6   | 2.41                     | 0.56              |
| 54:1:445:C:O2'   | 54:1:446:G:H5'   | 2.05                     | 0.56              |
| 54:1:519:U:H2'   | 54:1:520:G:H8    | 1.71                     | 0.56              |
| 54:1:796:C:H2'   | 54:1:797:G:H8    | 1.71                     | 0.56              |
| 54:1:1506:U:H2'  | 54:1:1507:C:C6   | 2.40                     | 0.56              |
| 54:1:1926:U:H2'  | 54:1:1928:A:OP2  | 2.06                     | 0.56              |
| 54:1:2297:A:N1   | 54:1:2321:U:C5   | 2.66                     | 0.56              |
| 54:1:2747:G:O6   | 54:1:2755:C:H5'' | 2.06                     | 0.56              |
| 56:5:18:G:H1     | 56:5:55:U:H6     | 1.54                     | 0.56              |
| 10:k:54:LYS:C    | 10:k:54:LYS:HD3  | 2.31                     | 0.56              |
| 11:l:78:ARG:NH2  | 11:l:78:ARG:HB3  | 2.20                     | 0.56              |
| 16:q:92:LYS:O    | 16:q:92:LYS:HD3  | 2.05                     | 0.56              |
| 30:E:62:PRO:HG2  | 30:E:63:TYR:CD2  | 2.41                     | 0.56              |
| 42:Q:114:SER:O   | 53:3:35:G:O2'    | 2.24                     | 0.56              |
| 50:Y:70:LYS:HA   | 50:Y:73:ARG:NH1  | 2.21                     | 0.56              |
| 53:3:830:G:H2'   | 53:3:831:A:C8    | 2.41                     | 0.56              |
| 54:1:270:A:H1'   | 54:1:370:G:N2    | 2.21                     | 0.56              |
| 54:1:644:A:H2'   | 54:1:645:C:C4'   | 2.36                     | 0.56              |
| 54:1:2134:A:N1   | 54:1:2157:G:H4'  | 2.21                     | 0.56              |
| 54:1:2333:A:H5'' | 54:1:2334:U:OP1  | 2.06                     | 0.56              |
| 54:1:2682:A:O2'  | 54:1:2683:C:H5'  | 2.06                     | 0.56              |
| 54:1:2834:G:O2'  | 54:1:2835:A:H5'  | 2.06                     | 0.56              |
| 1:b:107:LYS:N    | 1:b:193:GLU:O    | 2.39                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:e:35:LEU:HD21   | 4:e:56:LEU:HB3    | 1.87                     | 0.55              |
| 21:v:82:TYR:HE1   | 21:v:83:LYS:HE3   | 1.69                     | 0.55              |
| 27:B:39:ARG:HG3   | 27:B:40:HIS:CE1   | 2.41                     | 0.55              |
| 30:E:41:ARG:HA    | 30:E:44:ARG:HH11  | 1.71                     | 0.55              |
| 35:J:120:HIS:O    | 35:J:121:ASN:ND2  | 2.38                     | 0.55              |
| 35:J:156:ARG:HG3  | 38:M:43:GLY:O     | 2.04                     | 0.55              |
| 48:W:70:THR:HG23  | 48:W:72:ARG:H     | 1.71                     | 0.55              |
| 53:3:590:U:H2'    | 53:3:591:U:C6     | 2.41                     | 0.55              |
| 53:3:716:A:H2'    | 53:3:717:U:H6     | 1.70                     | 0.55              |
| 53:3:830:G:H2'    | 53:3:831:A:H8     | 1.70                     | 0.55              |
| 53:3:1390:U:H2'   | 53:3:1391:U:C6    | 2.41                     | 0.55              |
| 54:1:210:C:H2'    | 54:1:211:C:H6     | 1.71                     | 0.55              |
| 54:1:1775:U:C2'   | 54:1:1776:G:H5'   | 2.36                     | 0.55              |
| 59:8:167:VAL:O    | 59:8:169:LEU:HD12 | 2.06                     | 0.55              |
| 59:8:475:ARG:HH11 | 59:8:475:ARG:HA   | 1.71                     | 0.55              |
| 59:8:556:GLY:O    | 59:8:559:GLU:HG3  | 2.07                     | 0.55              |
| 4:e:149:ARG:HD3   | 4:e:149:ARG:N     | 2.17                     | 0.55              |
| 7:h:30:SER:O      | 54:1:1054:A:H4'   | 2.06                     | 0.55              |
| 12:m:4:PRO:HG3    | 12:m:68:PHE:CE2   | 2.41                     | 0.55              |
| 16:q:24:TYR:O     | 16:q:27:ARG:HB2   | 2.07                     | 0.55              |
| 21:v:4:ILE:HG12   | 21:v:50:MET:HE1   | 1.87                     | 0.55              |
| 29:D:30:VAL:O     | 29:D:34:ARG:HG2   | 2.06                     | 0.55              |
| 53:3:1026:G:N2    | 53:3:1027:C:H1'   | 2.20                     | 0.55              |
| 53:3:1450:U:H2'   | 53:3:1452:C:O4'   | 2.06                     | 0.55              |
| 54:1:131:A:H2'    | 54:1:132:G:H8     | 1.71                     | 0.55              |
| 54:1:743:A:O2'    | 54:1:744:U:H5'    | 2.06                     | 0.55              |
| 54:1:2798:U:H4'   | 54:1:2799:A:C4    | 2.40                     | 0.55              |
| 9:j:99:ARG:HH21   | 9:j:103:ILE:HD11  | 1.71                     | 0.55              |
| 15:p:96:LEU:O     | 15:p:99:LEU:HD23  | 2.07                     | 0.55              |
| 30:E:61:LEU:HD12  | 30:E:61:LEU:O     | 2.07                     | 0.55              |
| 34:I:10:LEU:HD13  | 34:I:62:ARG:HD2   | 1.89                     | 0.55              |
| 38:M:28:SER:HB3   | 38:M:56:PRO:HB2   | 1.88                     | 0.55              |
| 38:M:54:THR:HG23  | 38:M:55:LYS:HG3   | 1.87                     | 0.55              |
| 53:3:71:A:C2      | 53:3:100:G:H1'    | 2.40                     | 0.55              |
| 53:3:1487:G:O2'   | 53:3:1488:G:H5'   | 2.06                     | 0.55              |
| 54:1:679:C:H2'    | 54:1:680:C:H6     | 1.71                     | 0.55              |
| 54:1:2389:G:H5''  | 54:1:2390:U:O4'   | 2.06                     | 0.55              |
| 54:1:2557:G:H2'   | 54:1:2558:C:C6    | 2.40                     | 0.55              |
| 59:8:147:MET:HA   | 59:8:176:GLU:OE1  | 2.06                     | 0.55              |
| 3:d:106:LYS:HG3   | 3:d:200:LEU:HD11  | 1.87                     | 0.55              |
| 8:i:9:LYS:HE3     | 54:1:1070:A:N3    | 2.21                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:m:12:MET:HA   | 54:1:910:A:N6    | 2.12                     | 0.55              |
| 29:D:34:ARG:HD3  | 54:1:467:G:OP2   | 2.07                     | 0.55              |
| 37:L:2:ARG:HG3   | 53:3:1380:U:C4   | 2.41                     | 0.55              |
| 43:R:98:GLY:C    | 53:3:1308:U:OP2  | 2.50                     | 0.55              |
| 52:a:6:LYS:O     | 52:a:10:VAL:HG23 | 2.06                     | 0.55              |
| 53:3:376:G:H2'   | 53:3:377:G:H8    | 1.70                     | 0.55              |
| 2:c:161:MET:HE1  | 54:1:2050:C:O2   | 2.06                     | 0.55              |
| 3:d:57:LYS:HD3   | 3:d:58:LYS:O     | 2.07                     | 0.55              |
| 19:t:33:LYS:HG2  | 19:t:80:TRP:CZ3  | 2.42                     | 0.55              |
| 41:P:88:PRO:HG2  | 41:P:89:GLY:H    | 1.70                     | 0.55              |
| 43:R:3:ILE:HG22  | 43:R:4:ALA:H     | 1.71                     | 0.55              |
| 53:3:882:C:O2'   | 53:3:883:C:H5'   | 2.06                     | 0.55              |
| 53:3:940:C:H2'   | 53:3:941:G:C8    | 2.42                     | 0.55              |
| 2:c:2:ILE:HD13   | 2:c:90:PHE:CZ    | 2.42                     | 0.55              |
| 10:k:93:GLN:CD   | 10:k:93:GLN:H    | 2.14                     | 0.55              |
| 22:w:17:LEU:HD21 | 22:w:37:ARG:CZ   | 2.37                     | 0.55              |
| 32:G:60:ALA:HB1  | 32:G:223:GLY:HA3 | 1.89                     | 0.55              |
| 33:H:120:THR:O   | 33:H:124:GLU:HG2 | 2.07                     | 0.55              |
| 40:O:49:PHE:CE1  | 44:S:75:LYS:HG2  | 2.42                     | 0.55              |
| 51:Z:3:ILE:HD13  | 51:Z:19:LYS:HG2  | 1.88                     | 0.55              |
| 54:1:181:A:H2'   | 54:1:182:A:C8    | 2.42                     | 0.55              |
| 54:1:2070:A:H2'  | 54:1:2071:A:C8   | 2.41                     | 0.55              |
| 21:v:82:TYR:CE1  | 21:v:83:LYS:HG3  | 2.42                     | 0.55              |
| 26:A:2:LYS:HG3   | 55:2:40:U:C5     | 2.42                     | 0.55              |
| 26:A:56:ARG:HH12 | 53:3:1013:G:H5'' | 1.72                     | 0.55              |
| 41:P:21:HIS:ND1  | 41:P:84:MET:HB3  | 2.22                     | 0.55              |
| 43:R:18:LEU:O    | 43:R:21:ILE:HG22 | 2.06                     | 0.55              |
| 45:T:28:VAL:HG11 | 45:T:66:LEU:HD21 | 1.88                     | 0.55              |
| 48:W:54:LEU:C    | 48:W:54:LEU:HD12 | 2.32                     | 0.55              |
| 53:3:223:A:H2'   | 53:3:224:U:C6    | 2.42                     | 0.55              |
| 53:3:256:U:H2'   | 53:3:257:G:H8    | 1.72                     | 0.55              |
| 53:3:271:C:H2'   | 53:3:272:C:H6    | 1.71                     | 0.55              |
| 53:3:1166:G:N2   | 53:3:1168:U:OP1  | 2.35                     | 0.55              |
| 53:3:1383:C:HO2' | 53:3:1384:C:H6   | 1.54                     | 0.55              |
| 54:1:235:U:H2'   | 54:1:236:C:C6    | 2.42                     | 0.55              |
| 54:1:310:A:H2'   | 54:1:311:A:H5''  | 1.88                     | 0.55              |
| 54:1:1175:A:H5'' | 54:1:1176:U:H5'  | 1.88                     | 0.55              |
| 54:1:1199:U:H2'  | 54:1:1200:C:C6   | 2.42                     | 0.55              |
| 55:2:3:C:C3'     | 55:2:4:C:H5''    | 2.37                     | 0.55              |
| 59:8:87:ILE:HD12 | 59:8:87:ILE:N    | 2.21                     | 0.55              |
| 59:8:439:ALA:HA  | 59:8:442:ASP:OD1 | 2.07                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:j:37:ARG:HH22  | 9:j:110:PRO:HG3   | 1.71                     | 0.55              |
| 20:u:85:ARG:HG3  | 20:u:87:GLU:HG3   | 1.88                     | 0.55              |
| 21:v:75:GLN:HB2  | 21:v:92:VAL:N     | 2.22                     | 0.55              |
| 32:G:44:LYS:O    | 32:G:47:PRO:HD2   | 2.07                     | 0.55              |
| 34:I:169:TRP:O   | 34:I:182:LYS:HB2  | 2.06                     | 0.55              |
| 46:U:1:MET:CE    | 46:U:2:VAL:H      | 2.19                     | 0.55              |
| 53:3:936:C:H1'   | 53:3:1383:C:H41   | 1.71                     | 0.55              |
| 53:3:1280:A:H5'  | 53:3:1280:A:C8    | 2.41                     | 0.55              |
| 54:1:414:C:H2'   | 54:1:415:A:H8     | 1.71                     | 0.55              |
| 54:1:694:U:C3'   | 54:1:695:G:H5''   | 2.36                     | 0.55              |
| 54:1:1416:G:H2'  | 54:1:1417:C:C6    | 2.42                     | 0.55              |
| 54:1:1788:C:H2'  | 54:1:1789:A:H8    | 1.71                     | 0.55              |
| 54:1:2292:U:H2'  | 54:1:2293:G:C8    | 2.42                     | 0.55              |
| 59:8:13:ILE:HG21 | 59:8:286:LEU:HD23 | 1.87                     | 0.55              |
| 59:8:660:LEU:CD1 | 59:8:682:MET:HE1  | 2.37                     | 0.55              |
| 4:e:3:LEU:O      | 4:e:7:TYR:N       | 2.39                     | 0.55              |
| 8:i:56:VAL:HG23  | 8:i:70:THR:HA     | 1.89                     | 0.55              |
| 13:n:22:ARG:HG3  | 13:n:70:THR:HA    | 1.89                     | 0.55              |
| 13:n:49:GLU:HB2  | 13:n:50:PRO:HD3   | 1.89                     | 0.55              |
| 20:u:35:VAL:HG23 | 20:u:64:ILE:HG21  | 1.89                     | 0.55              |
| 24:y:47:ARG:NH2  | 54:1:60:G:H5''    | 2.22                     | 0.55              |
| 34:I:169:TRP:HB2 | 34:I:185:PRO:HG3  | 1.89                     | 0.55              |
| 53:3:1059:C:O2'  | 53:3:1060:U:H5'   | 2.07                     | 0.55              |
| 53:3:1269:A:H2   | 53:3:1312:G:H2'   | 1.72                     | 0.55              |
| 54:1:546:U:H2'   | 54:1:547:A:H4'    | 1.89                     | 0.55              |
| 54:1:1170:C:H2'  | 54:1:1171:G:N7    | 2.22                     | 0.55              |
| 54:1:1190:G:H2'  | 54:1:1191:G:H8    | 1.71                     | 0.55              |
| 54:1:1662:U:O2'  | 54:1:1663:G:H5'   | 2.07                     | 0.55              |
| 54:1:2515:C:H2'  | 54:1:2516:A:H8    | 1.71                     | 0.55              |
| 59:8:536:PHE:HA  | 59:8:576:ILE:O    | 2.07                     | 0.55              |
| 3:d:24:ASN:O     | 3:d:28:VAL:HG23   | 2.07                     | 0.55              |
| 8:i:55:PRO:HG2   | 8:i:71:LYS:HE2    | 1.88                     | 0.55              |
| 12:m:1:MET:HB3   | 12:m:43:ALA:HB1   | 1.89                     | 0.55              |
| 12:m:41:LEU:HD13 | 12:m:96:ILE:CG1   | 2.36                     | 0.55              |
| 14:o:85:LYS:HB2  | 14:o:87:ILE:CD1   | 2.37                     | 0.55              |
| 15:p:26:GLU:OE2  | 15:p:28:LYS:HG3   | 2.07                     | 0.55              |
| 18:s:18:ARG:NH2  | 54:1:518:G:H4'    | 2.22                     | 0.55              |
| 28:C:5:ARG:HH12  | 28:C:25:ASN:HB2   | 1.71                     | 0.55              |
| 35:J:92:ARG:O    | 35:J:93:VAL:C     | 2.48                     | 0.55              |
| 37:L:113:LYS:H   | 37:L:117:LEU:HD23 | 1.72                     | 0.55              |
| 38:M:26:MET:HE3  | 38:M:58:LEU:HD23  | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:N:29:ILE:N     | 39:N:29:ILE:HD12  | 2.22                     | 0.55              |
| 41:P:126:ARG:C    | 51:Z:34:ARG:HH21  | 2.15                     | 0.55              |
| 43:R:69:ARG:NH1   | 43:R:69:ARG:HB2   | 2.21                     | 0.55              |
| 44:S:62:ARG:HD2   | 44:S:67:GLY:O     | 2.06                     | 0.55              |
| 45:T:46:LYS:O     | 45:T:46:LYS:HG2   | 2.05                     | 0.55              |
| 49:X:21:ALA:O     | 49:X:25:GLY:N     | 2.37                     | 0.55              |
| 52:a:196:LEU:CD1  | 52:a:209:ILE:HD11 | 2.30                     | 0.55              |
| 53:3:15:G:H2'     | 53:3:16:A:H8      | 1.71                     | 0.55              |
| 54:1:2:G:N2       | 54:1:2902:C:H1'   | 2.21                     | 0.55              |
| 54:1:1038:G:H2'   | 54:1:1039:A:C8    | 2.42                     | 0.55              |
| 54:1:2638:G:H1'   | 54:1:2778:A:H61   | 1.72                     | 0.55              |
| 57:6:47:U:H5''    | 57:6:48:C:H5'     | 1.89                     | 0.55              |
| 59:8:84:ILE:HD12  | 59:8:84:ILE:N     | 2.22                     | 0.55              |
| 1:b:79:ARG:HE     | 1:b:92:LEU:HD22   | 1.72                     | 0.54              |
| 3:d:29:HIS:O      | 3:d:33:VAL:HG23   | 2.07                     | 0.54              |
| 5:f:86:LEU:HB2    | 5:f:130:ILE:HG23  | 1.89                     | 0.54              |
| 10:k:87:LEU:HB3   | 10:k:92:GLU:O     | 2.07                     | 0.54              |
| 11:l:23:ILE:HD12  | 11:l:23:ILE:N     | 2.14                     | 0.54              |
| 35:J:158:LYS:N    | 35:J:158:LYS:HD2  | 2.22                     | 0.54              |
| 39:N:112:ARG:NH2  | 53:3:1187:G:H4'   | 2.22                     | 0.54              |
| 50:Y:67:HIS:CG    | 53:3:262:A:H5'    | 2.42                     | 0.54              |
| 51:Z:38:GLU:C     | 51:Z:40:PRO:HD2   | 2.32                     | 0.54              |
| 53:3:15:G:C2      | 53:3:1080:A:H1'   | 2.42                     | 0.54              |
| 53:3:1270:G:H2'   | 53:3:1271:A:H8    | 1.71                     | 0.54              |
| 54:1:693:A:H2'    | 54:1:694:U:C6     | 2.42                     | 0.54              |
| 54:1:2799:A:H2'   | 54:1:2800:A:H5'   | 1.88                     | 0.54              |
| 59:8:56:GLU:HG3   | 59:8:61:ILE:O     | 2.06                     | 0.54              |
| 59:8:446:ARG:HH11 | 59:8:446:ARG:HG3  | 1.71                     | 0.54              |
| 3:d:145:ASP:HB2   | 3:d:184:ASP:H     | 1.72                     | 0.54              |
| 3:d:148:ILE:HB    | 3:d:169:VAL:HA    | 1.89                     | 0.54              |
| 3:d:164:LEU:HD23  | 3:d:167:VAL:HG21  | 1.89                     | 0.54              |
| 41:P:35:ASP:OD2   | 41:P:37:GLN:HB2   | 2.07                     | 0.54              |
| 50:Y:67:HIS:C     | 50:Y:69:ASN:H     | 2.15                     | 0.54              |
| 52:a:189:LEU:HD11 | 52:a:212:VAL:HG12 | 1.88                     | 0.54              |
| 53:3:560:A:H4'    | 53:3:561:U:H5'    | 1.90                     | 0.54              |
| 53:3:1090:U:O2    | 53:3:1095:U:O4    | 2.25                     | 0.54              |
| 53:3:1379:G:O2'   | 53:3:1380:U:H5'   | 2.06                     | 0.54              |
| 54:1:708:G:H2'    | 54:1:709:U:C6     | 2.42                     | 0.54              |
| 54:1:1086:A:H3'   | 54:1:1086:A:N3    | 2.22                     | 0.54              |
| 54:1:2126:A:H2'   | 54:1:2162:G:C2    | 2.42                     | 0.54              |
| 57:6:27:U:H2'     | 57:6:28:C:C5'     | 2.37                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 59:8:111:MET:CE   | 59:8:137:ARG:HD3  | 2.37                     | 0.54              |
| 59:8:342:VAL:HG12 | 59:8:378:ARG:HA   | 1.89                     | 0.54              |
| 4:e:166:ARG:CB    | 4:e:166:ARG:HH11  | 2.20                     | 0.54              |
| 5:f:42:VAL:HB     | 5:f:51:PHE:CE1    | 2.42                     | 0.54              |
| 10:k:103:VAL:HG23 | 10:k:104:THR:N    | 2.16                     | 0.54              |
| 12:m:78:LEU:HD23  | 12:m:79:ALA:HB2   | 1.88                     | 0.54              |
| 16:q:91:ARG:N     | 16:q:91:ARG:HD2   | 2.23                     | 0.54              |
| 32:G:199:ILE:HD12 | 32:G:199:ILE:N    | 2.22                     | 0.54              |
| 37:L:145:GLU:HA   | 37:L:148:LYS:HE3  | 1.90                     | 0.54              |
| 38:M:35:ILE:O     | 38:M:38:VAL:HG12  | 2.07                     | 0.54              |
| 50:Y:59:ARG:O     | 50:Y:63:LYS:HG2   | 2.06                     | 0.54              |
| 53:3:59:A:H5''    | 53:3:387:U:H5''   | 1.89                     | 0.54              |
| 53:3:1502:A:H8    | 53:3:1505:G:N2    | 1.97                     | 0.54              |
| 54:1:224:U:O4     | 54:1:420:C:H5'    | 2.08                     | 0.54              |
| 59:8:202:PHE:H    | 59:8:202:PHE:HD1  | 1.55                     | 0.54              |
| 59:8:366:MET:CE   | 59:8:371:ARG:HA   | 2.36                     | 0.54              |
| 59:8:497:LYS:HD3  | 59:8:523:TYR:CE1  | 2.43                     | 0.54              |
| 1:b:123:ILE:HG23  | 1:b:191:LEU:CD1   | 2.36                     | 0.54              |
| 1:b:204:LEU:HD12  | 1:b:209:ALA:HB1   | 1.90                     | 0.54              |
| 3:d:6:LYS:HB3     | 3:d:121:VAL:HG12  | 1.88                     | 0.54              |
| 6:g:5:LEU:HD13    | 6:g:13:GLY:CA     | 2.37                     | 0.54              |
| 10:k:104:THR:CG2  | 10:k:105:ARG:N    | 2.71                     | 0.54              |
| 10:k:111:LYS:HE3  | 10:k:112:PHE:CZ   | 2.43                     | 0.54              |
| 12:m:26:VAL:HB    | 12:m:133:LYS:HA   | 1.89                     | 0.54              |
| 14:o:43:ASN:ND2   | 14:o:45:SER:CB    | 2.70                     | 0.54              |
| 15:p:28:LYS:HD3   | 15:p:82:SER:OG    | 2.08                     | 0.54              |
| 15:p:85:VAL:HG12  | 15:p:86:LYS:N     | 2.22                     | 0.54              |
| 18:s:29:VAL:HG23  | 18:s:69:LEU:O     | 2.06                     | 0.54              |
| 38:M:107:LYS:H    | 38:M:120:LEU:HD11 | 1.73                     | 0.54              |
| 40:O:53:ILE:HD12  | 44:S:84:ARG:HD2   | 1.89                     | 0.54              |
| 40:O:53:ILE:HG22  | 40:O:61:ALA:O     | 2.08                     | 0.54              |
| 46:U:16:PHE:CE2   | 53:3:625:U:H4'    | 2.42                     | 0.54              |
| 53:3:609:A:H2'    | 53:3:610:U:H5'    | 1.89                     | 0.54              |
| 53:3:1058:G:H8    | 53:3:1058:G:O5'   | 1.91                     | 0.54              |
| 54:1:329:G:O4'    | 54:1:477:A:H1'    | 2.07                     | 0.54              |
| 54:1:1681:G:N3    | 54:1:1762:A:H2'   | 2.22                     | 0.54              |
| 54:1:2156:G:C2'   | 54:1:2157:G:H5'   | 2.37                     | 0.54              |
| 57:6:28:C:O2'     | 57:6:29:G:H5'     | 2.06                     | 0.54              |
| 59:8:309:ARG:HG2  | 59:8:339:TYR:HB3  | 1.89                     | 0.54              |
| 1:b:65:ASP:OD2    | 1:b:68:ARG:HD2    | 2.07                     | 0.54              |
| 1:b:110:LYS:HB2   | 1:b:113:ASP:OD2   | 2.07                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:d:120:VAL:HG13  | 3:d:188:MET:O     | 2.07                     | 0.54              |
| 25:z:16:LEU:H     | 25:z:16:LEU:CD2   | 2.13                     | 0.54              |
| 36:K:51:ILE:C     | 36:K:53:LYS:N     | 2.65                     | 0.54              |
| 44:S:80:ARG:HH11  | 44:S:80:ARG:HG3   | 1.73                     | 0.54              |
| 50:Y:67:HIS:O     | 50:Y:68:LYS:HB3   | 2.08                     | 0.54              |
| 52:a:6:LYS:HG2    | 52:a:7:ARG:N      | 2.22                     | 0.54              |
| 52:a:54:LYS:HE3   | 52:a:205:LYS:CD   | 2.38                     | 0.54              |
| 53:3:1185:G:O6    | 53:3:1186:G:N1    | 2.40                     | 0.54              |
| 53:3:1515:G:O2'   | 53:3:1516:G:H5'   | 2.07                     | 0.54              |
| 54:1:115:C:O2'    | 54:1:116:C:H5'    | 2.08                     | 0.54              |
| 54:1:2171:A:H5'   | 54:1:2174:C:H41   | 1.73                     | 0.54              |
| 54:1:2760:C:O2'   | 54:1:2761:A:H5'   | 2.07                     | 0.54              |
| 55:2:48:U:H2'     | 55:2:49:C:H6      | 1.73                     | 0.54              |
| 19:t:15:HIS:H     | 19:t:32:LEU:HA    | 1.71                     | 0.54              |
| 35:J:123:LEU:HD12 | 35:J:123:LEU:O    | 2.08                     | 0.54              |
| 36:K:60:VAL:HG12  | 36:K:62:MET:SD    | 2.48                     | 0.54              |
| 42:Q:93:ARG:HG3   | 42:Q:93:ARG:NH1   | 2.23                     | 0.54              |
| 43:R:97:ARG:NH1   | 53:3:1308:U:O2    | 2.41                     | 0.54              |
| 45:T:28:VAL:HG13  | 45:T:62:ARG:HD2   | 1.90                     | 0.54              |
| 48:W:49:LYS:O     | 48:W:53:GLN:HG3   | 2.08                     | 0.54              |
| 52:a:49:GLY:HA2   | 52:a:210:LYS:HZ2  | 1.72                     | 0.54              |
| 59:8:396:THR:HB   | 59:8:404:ILE:HG22 | 1.90                     | 0.54              |
| 1:b:211:ARG:HG2   | 1:b:211:ARG:HH11  | 1.73                     | 0.54              |
| 23:x:53:LYS:O     | 23:x:57:VAL:HG23  | 2.08                     | 0.54              |
| 33:H:102:ILE:HD12 | 33:H:102:ILE:N    | 2.22                     | 0.54              |
| 34:I:117:VAL:HG22 | 34:I:122:ILE:HG13 | 1.90                     | 0.54              |
| 37:L:73:GLU:HG2   | 37:L:74:VAL:N     | 2.21                     | 0.54              |
| 54:1:1034:G:H2'   | 54:1:1035:U:C6    | 2.43                     | 0.54              |
| 54:1:2443:C:O2'   | 54:1:2444:G:H5'   | 2.08                     | 0.54              |
| 54:1:2528:U:H2'   | 54:1:2530:A:O5'   | 2.08                     | 0.54              |
| 5:f:28:LYS:H      | 5:f:28:LYS:HD2    | 1.73                     | 0.54              |
| 26:A:62:LYS:HD3   | 49:X:16:LYS:HB3   | 1.90                     | 0.54              |
| 33:H:74:ILE:HD12  | 33:H:74:ILE:N     | 2.22                     | 0.54              |
| 35:J:156:ARG:HH22 | 38:M:42:GLU:HG3   | 1.71                     | 0.54              |
| 36:K:9:MET:HG3    | 36:K:86:ARG:O     | 2.07                     | 0.54              |
| 41:P:125:LYS:O    | 51:Z:34:ARG:NE    | 2.41                     | 0.54              |
| 42:Q:71:HIS:HB2   | 42:Q:73:LEU:HD13  | 1.90                     | 0.54              |
| 43:R:89:ARG:HG3   | 43:R:95:PRO:O     | 2.08                     | 0.54              |
| 49:X:49:ALA:HB1   | 49:X:56:HIS:HB3   | 1.89                     | 0.54              |
| 52:a:42:VAL:HG22  | 52:a:216:THR:HG22 | 1.90                     | 0.54              |
| 53:3:128:G:O2'    | 53:3:129:A:H5'    | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:3:455:G:H2'   | 53:3:456:A:H8    | 1.73                     | 0.54              |
| 53:3:664:G:H2'   | 53:3:666:G:OP1   | 2.07                     | 0.54              |
| 53:3:1121:U:OP2  | 53:3:1121:U:C6   | 2.60                     | 0.54              |
| 54:1:1306:C:H41  | 54:1:1606:C:H2'  | 1.72                     | 0.54              |
| 54:1:1689:A:H2'  | 54:1:1690:A:H8   | 1.73                     | 0.54              |
| 54:1:2114:A:H61  | 54:1:2117:A:H62  | 1.56                     | 0.54              |
| 54:1:2469:A:H2'  | 54:1:2470:G:O4'  | 2.08                     | 0.54              |
| 55:2:29:A:H2'    | 55:2:30:C:C6     | 2.43                     | 0.54              |
| 57:6:57:A:H2'    | 57:6:58:A:H5'    | 1.88                     | 0.54              |
| 2:c:161:MET:CE   | 54:1:2050:C:H1'  | 2.38                     | 0.54              |
| 6:g:118:PRO:HG2  | 6:g:130:VAL:HG13 | 1.87                     | 0.54              |
| 32:G:19:THR:OG1  | 32:G:20:ARG:HD3  | 2.08                     | 0.54              |
| 38:M:73:SER:N    | 38:M:129:ALA:O   | 2.39                     | 0.54              |
| 40:O:67:ILE:HG22 | 44:S:95:LEU:HA   | 1.90                     | 0.54              |
| 48:W:25:ILE:HA   | 48:W:28:LEU:HD12 | 1.89                     | 0.54              |
| 49:X:53:GLY:HA2  | 53:3:1221:G:H4'  | 1.88                     | 0.54              |
| 53:3:946:A:C4    | 53:3:947:G:C8    | 2.96                     | 0.54              |
| 53:3:1091:U:C5   | 53:3:1092:A:H3'  | 2.43                     | 0.54              |
| 53:3:1333:A:H2'  | 53:3:1334:G:O4'  | 2.07                     | 0.54              |
| 54:1:1198:U:H2'  | 54:1:1199:U:C6   | 2.43                     | 0.54              |
| 54:1:1563:U:H2'  | 54:1:1564:C:C6   | 2.42                     | 0.54              |
| 54:1:2519:U:H5'  | 54:1:2567:G:H21  | 1.71                     | 0.54              |
| 59:8:399:ASP:CG  | 59:8:400:PRO:HD3 | 2.33                     | 0.54              |
| 2:c:108:ASP:OD1  | 2:c:206:ALA:HA   | 2.08                     | 0.54              |
| 4:e:116:LEU:HB2  | 4:e:175:PRO:HB2  | 1.90                     | 0.54              |
| 4:e:122:ASP:OD2  | 4:e:124:ARG:HB3  | 2.08                     | 0.54              |
| 8:i:12:VAL:HA    | 54:1:1061:U:N3   | 2.16                     | 0.54              |
| 17:r:83:TYR:HE1  | 17:r:85:LYS:HE2  | 1.73                     | 0.54              |
| 19:t:24:MET:O    | 19:t:28:ASN:HA   | 2.08                     | 0.54              |
| 28:C:37:LYS:HG2  | 54:1:2345:G:OP2  | 2.08                     | 0.54              |
| 33:H:4:VAL:HG22  | 33:H:5:HIS:N     | 2.23                     | 0.54              |
| 35:J:82:HIS:HB2  | 35:J:83:PRO:HD2  | 1.89                     | 0.54              |
| 35:J:104:ILE:HA  | 35:J:121:ASN:O   | 2.08                     | 0.54              |
| 36:K:27:ALA:O    | 36:K:31:GLY:N    | 2.40                     | 0.54              |
| 36:K:100:SER:OG  | 48:W:23:LYS:HE3  | 2.07                     | 0.54              |
| 44:S:9:GLU:O     | 44:S:13:VAL:HG23 | 2.08                     | 0.54              |
| 47:V:37:ILE:HG13 | 47:V:38:LYS:H    | 1.71                     | 0.54              |
| 51:Z:36:PHE:O    | 51:Z:38:GLU:N    | 2.40                     | 0.54              |
| 51:Z:52:VAL:O    | 51:Z:56:ALA:N    | 2.40                     | 0.54              |
| 53:3:15:G:O6     | 53:3:1080:A:N3   | 2.41                     | 0.54              |
| 53:3:1357:A:H2   | 53:3:1365:G:H22  | 1.56                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:1514:G:O2'   | 53:3:1515:G:H5'   | 2.07                     | 0.54              |
| 54:1:1609:A:H1'   | 54:1:1616:A:C1'   | 2.38                     | 0.54              |
| 54:1:1789:A:H2'   | 54:1:1790:C:O4'   | 2.07                     | 0.54              |
| 59:8:107:ASP:O    | 59:8:136:PRO:HD2  | 2.07                     | 0.54              |
| 5:f:86:LEU:HB2    | 5:f:130:ILE:CG2   | 2.37                     | 0.53              |
| 6:g:1:MET:HG3     | 6:g:3:VAL:HG23    | 1.90                     | 0.53              |
| 14:o:4:LYS:HE3    | 14:o:7:ARG:HH21   | 1.72                     | 0.53              |
| 26:A:56:ARG:NH1   | 53:3:1013:G:H5'   | 2.24                     | 0.53              |
| 32:G:47:PRO:O     | 32:G:51:GLU:HG3   | 2.08                     | 0.53              |
| 32:G:134:LEU:HD12 | 32:G:135:MET:N    | 2.23                     | 0.53              |
| 39:N:5:TYR:HB2    | 39:N:20:ILE:HG22  | 1.90                     | 0.53              |
| 48:W:47:ARG:HB2   | 48:W:50:TYR:HD2   | 1.73                     | 0.53              |
| 50:Y:34:VAL:HG22  | 50:Y:49:ALA:HB1   | 1.90                     | 0.53              |
| 53:3:402:G:O2'    | 53:3:403:C:H5'    | 2.08                     | 0.53              |
| 53:3:1236:A:H2'   | 53:3:1237:C:C6    | 2.44                     | 0.53              |
| 53:3:1302:C:O2'   | 53:3:1303:C:C5'   | 2.56                     | 0.53              |
| 53:3:1511:G:O2'   | 53:3:1512:U:H5'   | 2.08                     | 0.53              |
| 54:1:3:U:H2'      | 54:1:4:U:C6       | 2.43                     | 0.53              |
| 54:1:214:G:H2'    | 54:1:215:G:C8     | 2.43                     | 0.53              |
| 54:1:1278:C:H2'   | 54:1:1279:G:C8    | 2.43                     | 0.53              |
| 54:1:2625:G:H2'   | 54:1:2626:C:C6    | 2.43                     | 0.53              |
| 59:8:61:ILE:HB    | 59:8:92:HIS:CE1   | 2.42                     | 0.53              |
| 2:c:129:THR:HG22  | 2:c:130:GLN:O     | 2.07                     | 0.53              |
| 7:h:60:LEU:HD23   | 7:h:60:LEU:H      | 1.73                     | 0.53              |
| 13:n:59:SER:O     | 13:n:63:ARG:HG2   | 2.08                     | 0.53              |
| 14:o:47:VAL:HG21  | 55:2:114:C:H4'    | 1.88                     | 0.53              |
| 21:v:72:VAL:HA    | 21:v:94:ALA:H     | 1.73                     | 0.53              |
| 33:H:153:SER:HA   | 33:H:164:THR:HG22 | 1.89                     | 0.53              |
| 34:I:183:ARG:HG2  | 34:I:183:ARG:HH11 | 1.72                     | 0.53              |
| 35:J:131:ASN:O    | 35:J:135:VAL:HG23 | 2.08                     | 0.53              |
| 53:3:636:U:H2'    | 53:3:637:C:H6     | 1.73                     | 0.53              |
| 53:3:781:A:OP1    | 53:3:1523:G:H5'   | 2.08                     | 0.53              |
| 53:3:1060:U:C2'   | 53:3:1061:G:H5'   | 2.38                     | 0.53              |
| 53:3:1341:U:O2'   | 53:3:1342:C:H5'   | 2.09                     | 0.53              |
| 54:1:1040:A:O2'   | 54:1:1041:G:H5'   | 2.08                     | 0.53              |
| 54:1:1308:A:C2'   | 54:1:1309:G:H5'   | 2.38                     | 0.53              |
| 54:1:1796:U:H2'   | 54:1:1797:G:C8    | 2.43                     | 0.53              |
| 59:8:346:GLY:HA2  | 59:8:360:PHE:O    | 2.07                     | 0.53              |
| 3:d:5:LEU:O       | 3:d:9:GLN:HA      | 2.09                     | 0.53              |
| 11:l:36:LYS:HD3   | 54:1:807:U:OP2    | 2.09                     | 0.53              |
| 11:l:101:ILE:HG13 | 11:l:102:GLY:H    | 1.73                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:x:35:HIS:CB    | 23:x:55:MET:HE1   | 2.38                     | 0.53              |
| 35:J:15:ILE:HD12  | 35:J:15:ILE:N     | 2.22                     | 0.53              |
| 35:J:93:VAL:CG1   | 35:J:110:MET:HE1  | 2.38                     | 0.53              |
| 37:L:91:ARG:HG2   | 37:L:91:ARG:HH11  | 1.73                     | 0.53              |
| 38:M:9:MET:HB2    | 38:M:32:LYS:HE2   | 1.90                     | 0.53              |
| 39:N:17:ARG:NH1   | 53:3:1129:C:H4'   | 2.23                     | 0.53              |
| 54:1:492:A:H2'    | 54:1:493:G:O4'    | 2.08                     | 0.53              |
| 54:1:543:G:H2'    | 54:1:544:C:O4'    | 2.08                     | 0.53              |
| 54:1:1019:U:H2'   | 54:1:1020:A:C8    | 2.42                     | 0.53              |
| 54:1:2737:G:H2'   | 54:1:2738:A:C8    | 2.44                     | 0.53              |
| 59:8:519:VAL:HG22 | 59:8:580:PHE:O    | 2.08                     | 0.53              |
| 1:b:132:ARG:HG3   | 1:b:133:ASN:OD1   | 2.09                     | 0.53              |
| 3:d:63:LYS:HE2    | 54:1:2444:G:OP2   | 2.09                     | 0.53              |
| 13:n:4:ARG:HH21   | 54:1:2874:C:H5''  | 1.73                     | 0.53              |
| 24:y:19:LEU:HB3   | 24:y:23:ARG:HH12  | 1.73                     | 0.53              |
| 31:F:27:CYS:HB2   | 31:F:33:HIS:HB2   | 1.91                     | 0.53              |
| 41:P:125:LYS:HE3  | 53:3:797:C:OP1    | 2.09                     | 0.53              |
| 43:R:26:LYS:HE2   | 43:R:30:LYS:HE3   | 1.91                     | 0.53              |
| 46:U:65:ALA:O     | 46:U:67:ILE:HD12  | 2.09                     | 0.53              |
| 51:Z:11:PHE:C     | 51:Z:13:VAL:H     | 2.16                     | 0.53              |
| 53:3:370:C:H2'    | 53:3:371:A:C8     | 2.43                     | 0.53              |
| 53:3:533:A:O2'    | 53:3:534:U:H5''   | 2.08                     | 0.53              |
| 53:3:964:A:C5'    | 53:3:1199:U:OP1   | 2.56                     | 0.53              |
| 53:3:1404:C:H2'   | 53:3:1405:G:C8    | 2.44                     | 0.53              |
| 54:1:1536:C:H4'   | 54:1:1537:G:C2    | 2.43                     | 0.53              |
| 54:1:2185:U:H2'   | 54:1:2186:G:H8    | 1.72                     | 0.53              |
| 54:1:2185:U:H2'   | 54:1:2186:G:C8    | 2.42                     | 0.53              |
| 59:8:15:ILE:HD12  | 59:8:15:ILE:H     | 1.74                     | 0.53              |
| 59:8:465:HIS:O    | 59:8:469:ILE:HG13 | 2.08                     | 0.53              |
| 4:e:147:ARG:HD3   | 4:e:148:VAL:N     | 2.23                     | 0.53              |
| 6:g:25:TYR:O      | 6:g:30:LEU:HG     | 2.09                     | 0.53              |
| 10:k:36:GLY:HA2   | 10:k:62:VAL:O     | 2.09                     | 0.53              |
| 22:w:55:LEU:CD1   | 22:w:76:ILE:HD12  | 2.39                     | 0.53              |
| 24:y:6:LEU:HD13   | 24:y:56:LEU:HD22  | 1.89                     | 0.53              |
| 26:A:11:GLU:HB2   | 26:A:25:ARG:HD2   | 1.90                     | 0.53              |
| 34:I:152:SER:CB   | 53:3:436:C:H4'    | 2.36                     | 0.53              |
| 39:N:127:SER:HB2  | 53:3:1232:U:OP1   | 2.08                     | 0.53              |
| 43:R:72:ILE:O     | 43:R:76:ILE:HG13  | 2.08                     | 0.53              |
| 44:S:31:SER:HA    | 44:S:40:ARG:HG2   | 1.90                     | 0.53              |
| 53:3:77:A:H2'     | 53:3:78:A:H8      | 1.73                     | 0.53              |
| 53:3:879:C:H2'    | 53:3:880:C:H6     | 1.73                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:1011:C:H2'   | 53:3:1012:A:C8    | 2.43                     | 0.53              |
| 53:3:1328:C:H2'   | 53:3:1329:A:C8    | 2.44                     | 0.53              |
| 54:1:1070:A:H3'   | 54:1:1072:C:OP2   | 2.08                     | 0.53              |
| 54:1:1102:C:H2'   | 54:1:1103:A:C8    | 2.44                     | 0.53              |
| 54:1:1994:C:O2'   | 54:1:1995:U:H5'   | 2.07                     | 0.53              |
| 54:1:2291:U:H2'   | 54:1:2292:U:C6    | 2.44                     | 0.53              |
| 54:1:2805:C:H2'   | 54:1:2806:C:H6    | 1.74                     | 0.53              |
| 59:8:184:ASP:N    | 59:8:189:LYS:O    | 2.42                     | 0.53              |
| 3:d:176:ASP:O     | 3:d:180:LEU:HD23  | 2.09                     | 0.53              |
| 7:h:81:LEU:HD21   | 54:1:1106:G:H21   | 1.72                     | 0.53              |
| 10:k:13:ASN:ND2   | 10:k:98:ARG:HB3   | 2.21                     | 0.53              |
| 11:l:109:LYS:HG2  | 11:l:126:ARG:HB2  | 1.90                     | 0.53              |
| 13:n:8:ARG:HG3    | 13:n:8:ARG:HH21   | 1.73                     | 0.53              |
| 33:H:73:GLY:O     | 33:H:77:GLY:N     | 2.37                     | 0.53              |
| 47:V:11:VAL:HG22  | 47:V:22:VAL:HG12  | 1.90                     | 0.53              |
| 53:3:16:A:C2      | 53:3:1080:A:C5    | 2.96                     | 0.53              |
| 53:3:1233:G:H2'   | 53:3:1234:C:H6    | 1.74                     | 0.53              |
| 53:3:1371:G:H2'   | 53:3:1372:U:C6    | 2.44                     | 0.53              |
| 53:3:1399:C:H1'   | 53:3:1401:G:C8    | 2.44                     | 0.53              |
| 54:1:441:U:H2'    | 54:1:442:G:C8     | 2.43                     | 0.53              |
| 54:1:519:U:H2'    | 54:1:520:G:C8     | 2.43                     | 0.53              |
| 54:1:720:U:H2'    | 54:1:721:A:H8     | 1.74                     | 0.53              |
| 54:1:1412:U:H2'   | 54:1:1413:A:H8    | 1.72                     | 0.53              |
| 54:1:1857:G:N2    | 54:1:1884:G:H2'   | 2.23                     | 0.53              |
| 59:8:498:VAL:HG11 | 59:8:522:MET:HG2  | 1.91                     | 0.53              |
| 4:e:114:ARG:HD2   | 26:A:50:ASP:HB2   | 1.90                     | 0.53              |
| 18:s:6:LYS:HB2    | 18:s:103:ILE:O    | 2.08                     | 0.53              |
| 30:E:62:PRO:HG2   | 30:E:63:TYR:H     | 1.73                     | 0.53              |
| 30:E:63:TYR:CE2   | 54:1:242:G:H5''   | 2.43                     | 0.53              |
| 36:K:37:HIS:HB3   | 36:K:97:THR:HG21  | 1.91                     | 0.53              |
| 50:Y:23:ARG:HA    | 50:Y:23:ARG:HE    | 1.73                     | 0.53              |
| 53:3:946:A:H2'    | 53:3:947:G:H8     | 1.74                     | 0.53              |
| 53:3:1166:G:C8    | 53:3:1166:G:OP2   | 2.62                     | 0.53              |
| 54:1:1117:C:O2'   | 54:1:1118:C:H5'   | 2.08                     | 0.53              |
| 54:1:1361:G:H2'   | 54:1:1362:C:H6    | 1.72                     | 0.53              |
| 54:1:2163:A:C3'   | 54:1:2164:C:H5'   | 2.39                     | 0.53              |
| 59:8:337:ARG:HG3  | 59:8:382:ILE:HG22 | 1.90                     | 0.53              |
| 59:8:423:LYS:O    | 59:8:427:ASP:HB2  | 2.08                     | 0.53              |
| 15:p:52:ARG:HH21  | 54:1:2720:U:H5''  | 1.73                     | 0.53              |
| 34:I:15:GLY:HA2   | 34:I:34:GLU:HG3   | 1.91                     | 0.53              |
| 37:L:112:ASP:HB3  | 37:L:117:LEU:CD2  | 2.32                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 40:O:8:ILE:HD12  | 40:O:8:ILE:N      | 2.23                     | 0.53              |
| 42:Q:112:ALA:HB1 | 42:Q:115:LYS:HZ1  | 1.74                     | 0.53              |
| 53:3:15:G:H22    | 53:3:1080:A:C2'   | 2.21                     | 0.53              |
| 53:3:558:G:H2'   | 53:3:559:A:C2     | 2.44                     | 0.53              |
| 54:1:546:U:H2'   | 54:1:547:A:C4'    | 2.39                     | 0.53              |
| 54:1:577:G:H2'   | 54:1:578:G:C8     | 2.44                     | 0.53              |
| 54:1:656:G:H2'   | 54:1:657:U:C6     | 2.43                     | 0.53              |
| 54:1:974:G:N3    | 54:1:974:G:H2'    | 2.24                     | 0.53              |
| 54:1:1181:U:H2'  | 54:1:1182:G:H8    | 1.73                     | 0.53              |
| 54:1:1689:A:H2'  | 54:1:1690:A:C8    | 2.44                     | 0.53              |
| 54:1:2544:G:O2'  | 54:1:2545:G:H5'   | 2.09                     | 0.53              |
| 57:6:13:C:C2'    | 57:6:14:A:H5''    | 2.39                     | 0.53              |
| 1:b:144:GLU:HA   | 1:b:151:GLY:HA2   | 1.90                     | 0.53              |
| 3:d:68:ALA:HA    | 54:1:1255:U:C6    | 2.43                     | 0.53              |
| 3:d:117:ARG:HB3  | 3:d:184:ASP:O     | 2.08                     | 0.53              |
| 4:e:37:MET:HE1   | 4:e:150:GLY:O     | 2.08                     | 0.53              |
| 7:h:41:LEU:O     | 7:h:45:GLY:N      | 2.41                     | 0.53              |
| 8:i:37:PHE:HA    | 8:i:66:PHE:HE2    | 1.74                     | 0.53              |
| 10:k:25:LEU:HD23 | 10:k:39:ILE:HA    | 1.90                     | 0.53              |
| 16:q:23:TYR:CD1  | 54:1:533:G:H5'    | 2.43                     | 0.53              |
| 17:r:37:GLU:O    | 17:r:39:LEU:HD12  | 2.09                     | 0.53              |
| 23:x:28:PHE:HD1  | 54:1:396:G:H1'    | 1.74                     | 0.53              |
| 32:G:8:MET:HG2   | 32:G:10:LYS:HG2   | 1.90                     | 0.53              |
| 34:I:119:HIS:HB3 | 53:3:438:U:H5'    | 1.91                     | 0.53              |
| 36:K:12:PRO:HA   | 36:K:15:SER:OG    | 2.08                     | 0.53              |
| 37:L:94:ARG:O    | 37:L:97:ALA:HB3   | 2.08                     | 0.53              |
| 49:X:41:PRO:HA   | 49:X:44:ILE:HG13  | 1.91                     | 0.53              |
| 51:Z:11:PHE:O    | 51:Z:13:VAL:HG12  | 2.09                     | 0.53              |
| 53:3:114:U:H2'   | 53:3:115:G:C8     | 2.44                     | 0.53              |
| 53:3:131:A:H2'   | 53:3:132:C:H6     | 1.73                     | 0.53              |
| 54:1:796:C:H2'   | 54:1:797:G:C8     | 2.44                     | 0.53              |
| 54:1:799:G:H3'   | 54:1:800:A:H8     | 1.73                     | 0.53              |
| 54:1:1609:A:H1'  | 54:1:1616:A:H1'   | 1.91                     | 0.53              |
| 54:1:1682:G:H2'  | 54:1:1683:U:C6    | 2.44                     | 0.53              |
| 54:1:2386:A:H2'  | 54:1:2387:U:H6    | 1.74                     | 0.53              |
| 59:8:171:LEU:O   | 59:8:183:VAL:HG12 | 2.08                     | 0.53              |
| 59:8:599:ILE:N   | 59:8:599:ILE:HD12 | 2.24                     | 0.53              |
| 15:p:63:ILE:HA   | 15:p:68:GLY:HA2   | 1.91                     | 0.53              |
| 33:H:168:ARG:HG3 | 33:H:172:VAL:HG21 | 1.91                     | 0.53              |
| 34:I:8:LEU:HB3   | 53:3:430:A:OP1    | 2.08                     | 0.53              |
| 37:L:38:ALA:O    | 37:L:42:VAL:HG23  | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:M:31:LEU:O     | 38:M:35:ILE:HG12  | 2.09                     | 0.53              |
| 43:R:97:ARG:HA    | 53:3:1308:U:C1'   | 2.38                     | 0.53              |
| 53:3:381:C:H2'    | 53:3:382:A:O4'    | 2.09                     | 0.53              |
| 53:3:880:C:H2'    | 53:3:881:G:H8     | 1.74                     | 0.53              |
| 53:3:924:C:H4'    | 53:3:1399:C:C5'   | 2.39                     | 0.53              |
| 53:3:1328:C:H2'   | 53:3:1329:A:H8    | 1.73                     | 0.53              |
| 54:1:488:G:N2     | 54:1:491:G:H5''   | 2.23                     | 0.53              |
| 54:1:720:U:H2'    | 54:1:721:A:C8     | 2.43                     | 0.53              |
| 54:1:1074:G:H2'   | 54:1:1075:C:O4'   | 2.09                     | 0.53              |
| 54:1:1773:A:H2'   | 54:1:1774:C:C5'   | 2.39                     | 0.53              |
| 59:8:75:MET:HG3   | 59:8:79:TYR:CB    | 2.33                     | 0.53              |
| 1:b:242:HIS:O     | 1:b:244:VAL:HG13  | 2.08                     | 0.52              |
| 10:k:35:VAL:HG22  | 10:k:69:VAL:CG1   | 2.39                     | 0.52              |
| 11:l:95:LEU:HD22  | 11:l:100:ILE:CD1  | 2.39                     | 0.52              |
| 13:n:46:ARG:NH2   | 13:n:46:ARG:HB3   | 2.23                     | 0.52              |
| 13:n:73:ASN:O     | 13:n:76:VAL:HG12  | 2.08                     | 0.52              |
| 15:p:28:LYS:HE2   | 15:p:39:LEU:HD21  | 1.91                     | 0.52              |
| 16:q:29:ARG:HG3   | 16:q:29:ARG:NH1   | 2.23                     | 0.52              |
| 17:r:74:ILE:HB    | 17:r:87:GLN:HE21  | 1.74                     | 0.52              |
| 30:E:63:TYR:CZ    | 54:1:242:G:H5''   | 2.44                     | 0.52              |
| 31:F:23:ILE:HD13  | 31:F:38:GLY:OXT   | 2.09                     | 0.52              |
| 44:S:15:LEU:HD21  | 44:S:54:SER:HA    | 1.91                     | 0.52              |
| 51:Z:23:GLU:HG2   | 51:Z:24:LYS:H     | 1.73                     | 0.52              |
| 53:3:604:G:H2'    | 53:3:605:U:O4'    | 2.09                     | 0.52              |
| 53:3:976:G:H2'    | 53:3:1362:A:N1    | 2.24                     | 0.52              |
| 53:3:1101:A:H4'   | 53:3:1102:A:O5'   | 2.09                     | 0.52              |
| 53:3:1164:G:H21   | 53:3:1165:U:H3    | 1.57                     | 0.52              |
| 54:1:679:C:H2'    | 54:1:680:C:C6     | 2.43                     | 0.52              |
| 55:2:2:G:H2'      | 55:2:3:C:C6       | 2.44                     | 0.52              |
| 58:4:18:G:C3'     | 58:4:19:C:H5''    | 2.38                     | 0.52              |
| 59:8:153:LYS:O    | 59:8:157:GLN:HG2  | 2.10                     | 0.52              |
| 59:8:387:GLY:C    | 59:8:388:LEU:HD12 | 2.34                     | 0.52              |
| 1:b:83:ASP:OD2    | 1:b:86:ARG:HG2    | 2.09                     | 0.52              |
| 1:b:177:SER:OG    | 54:1:1799:G:N7    | 2.42                     | 0.52              |
| 3:d:113:VAL:HG22  | 3:d:118:LEU:HD23  | 1.91                     | 0.52              |
| 5:f:89:VAL:CG2    | 5:f:162:ARG:HE    | 2.23                     | 0.52              |
| 12:m:19:GLY:C     | 12:m:20:LEU:HD22  | 2.34                     | 0.52              |
| 15:p:113:LEU:HD11 | 53:3:1441:A:C2    | 2.44                     | 0.52              |
| 30:E:37:THR:HG21  | 54:1:2348:U:OP2   | 2.10                     | 0.52              |
| 34:I:84:ASN:HB2   | 34:I:87:GLU:HG2   | 1.90                     | 0.52              |
| 42:Q:55:ARG:C     | 42:Q:56:LEU:HD12  | 2.35                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:R:106:ARG:HG2  | 53:3:947:G:OP1    | 2.09                     | 0.52              |
| 53:3:801:U:H2'    | 53:3:802:A:H8     | 1.74                     | 0.52              |
| 53:3:1172:C:H2'   | 53:3:1173:U:C6    | 2.44                     | 0.52              |
| 54:1:287:G:H2'    | 54:1:288:U:C6     | 2.44                     | 0.52              |
| 54:1:1079:C:H2'   | 54:1:1080:A:H8    | 1.73                     | 0.52              |
| 54:1:2636:C:H2'   | 54:1:2637:U:C6    | 2.45                     | 0.52              |
| 54:1:2731:G:H2'   | 54:1:2732:G:C8    | 2.44                     | 0.52              |
| 59:8:6:PRO:HB3    | 59:8:9:ARG:HH21   | 1.74                     | 0.52              |
| 59:8:349:VAL:HG11 | 59:8:360:PHE:HE2  | 1.75                     | 0.52              |
| 59:8:349:VAL:CA   | 59:8:399:ASP:HB3  | 2.27                     | 0.52              |
| 5:f:14:VAL:CG1    | 5:f:25:ILE:HG23   | 2.40                     | 0.52              |
| 6:g:12:LEU:N      | 6:g:12:LEU:HD23   | 2.24                     | 0.52              |
| 10:k:12:ASP:OD2   | 10:k:14:SER:HB3   | 2.09                     | 0.52              |
| 18:s:82:MET:CB    | 18:s:84:ARG:HH22  | 2.19                     | 0.52              |
| 30:E:31:ILE:HD11  | 54:1:2391:G:H5'   | 1.90                     | 0.52              |
| 32:G:94:ARG:HH22  | 32:G:145:ASN:ND2  | 2.07                     | 0.52              |
| 36:K:94:HIS:O     | 36:K:96:VAL:HG13  | 2.09                     | 0.52              |
| 43:R:8:ILE:HD12   | 43:R:8:ILE:N      | 2.25                     | 0.52              |
| 45:T:50:HIS:ND1   | 53:3:667:G:H4'    | 2.25                     | 0.52              |
| 50:Y:2:ASN:ND2    | 50:Y:3:ILE:H      | 2.08                     | 0.52              |
| 51:Z:44:ARG:HD2   | 51:Z:44:ARG:C     | 2.33                     | 0.52              |
| 53:3:1126:U:H1'   | 53:3:1281:C:C5    | 2.45                     | 0.52              |
| 53:3:1185:G:C6    | 53:3:1186:G:C2    | 2.97                     | 0.52              |
| 54:1:1053:C:H3'   | 54:1:1054:A:H5''  | 1.90                     | 0.52              |
| 54:1:2493:U:H2'   | 54:1:2494:G:H5''  | 1.91                     | 0.52              |
| 54:1:2572:A:OP1   | 54:1:2574:G:H4'   | 2.09                     | 0.52              |
| 54:1:2869:G:H2'   | 54:1:2870:C:C6    | 2.44                     | 0.52              |
| 55:2:60:C:H2'     | 55:2:61:G:H8      | 1.74                     | 0.52              |
| 56:5:9:A:H5''     | 56:5:46:G:H1'     | 1.89                     | 0.52              |
| 59:8:628:THR:O    | 59:8:632:ILE:HG13 | 2.09                     | 0.52              |
| 3:d:148:ILE:HG21  | 3:d:157:LEU:HD21  | 1.91                     | 0.52              |
| 15:p:85:VAL:HG12  | 15:p:86:LYS:H     | 1.75                     | 0.52              |
| 17:r:74:ILE:N     | 17:r:74:ILE:HD12  | 2.24                     | 0.52              |
| 36:K:3:HIS:H      | 36:K:92:THR:CG2   | 2.17                     | 0.52              |
| 39:N:26:LYS:C     | 39:N:27:ILE:HD12  | 2.35                     | 0.52              |
| 44:S:48:GLN:HB2   | 49:X:12:LEU:HD11  | 1.90                     | 0.52              |
| 50:Y:66:ILE:HG22  | 50:Y:68:LYS:N     | 2.23                     | 0.52              |
| 53:3:490:C:H2'    | 53:3:491:G:H8     | 1.75                     | 0.52              |
| 53:3:854:U:H3'    | 53:3:871:U:H3     | 1.75                     | 0.52              |
| 53:3:1164:G:N2    | 53:3:1165:U:O4    | 2.43                     | 0.52              |
| 53:3:1412:C:H2'   | 53:3:1413:A:H8    | 1.72                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:741:U:H2'    | 54:1:742:A:H8     | 1.75                     | 0.52              |
| 54:1:876:C:H2'    | 54:1:877:A:O4'    | 2.09                     | 0.52              |
| 54:1:1396:U:H5''  | 54:1:1397:U:OP2   | 2.09                     | 0.52              |
| 59:8:6:PRO:CB     | 59:8:9:ARG:HE     | 2.21                     | 0.52              |
| 4:e:57:ALA:HB2    | 4:e:64:PRO:HD3    | 1.92                     | 0.52              |
| 11:l:3:LEU:HD23   | 54:1:1203:U:H5'   | 1.91                     | 0.52              |
| 23:x:2:ARG:NH1    | 54:1:1364:G:H5''  | 2.25                     | 0.52              |
| 49:X:36:ARG:NH1   | 53:3:1318:A:H1'   | 2.24                     | 0.52              |
| 54:1:546:U:H1'    | 54:1:548:G:C6     | 2.44                     | 0.52              |
| 54:1:1131:G:C8    | 54:1:2025:C:H4'   | 2.44                     | 0.52              |
| 54:1:1152:C:H2'   | 54:1:1153:C:H6    | 1.73                     | 0.52              |
| 54:1:2455:G:H2'   | 54:1:2456:C:C6    | 2.44                     | 0.52              |
| 59:8:353:VAL:HA   | 59:8:404:ILE:HD13 | 1.91                     | 0.52              |
| 59:8:553:VAL:HG12 | 59:8:593:PHE:HB3  | 1.91                     | 0.52              |
| 59:8:574:MET:HE1  | 59:8:601:PHE:HE1  | 1.75                     | 0.52              |
| 1:b:270:ARG:HH11  | 1:b:270:ARG:CB    | 2.18                     | 0.52              |
| 2:c:149:ASN:HB3   | 54:1:2572:A:OP2   | 2.09                     | 0.52              |
| 11:l:79:LEU:HB2   | 11:l:114:GLY:O    | 2.10                     | 0.52              |
| 18:s:47:VAL:O     | 18:s:50:VAL:HG12  | 2.09                     | 0.52              |
| 39:N:11:ARG:HH11  | 39:N:12:LYS:HB2   | 1.74                     | 0.52              |
| 52:a:7:ARG:NH2    | 52:a:11:ILE:HD11  | 2.25                     | 0.52              |
| 53:3:15:G:C6      | 53:3:1080:A:N3    | 2.77                     | 0.52              |
| 53:3:1184:G:N3    | 53:3:1184:G:H2'   | 2.25                     | 0.52              |
| 53:3:1381:U:H4'   | 53:3:1535:C:O2'   | 2.09                     | 0.52              |
| 54:1:78:U:H2'     | 54:1:79:C:C6      | 2.44                     | 0.52              |
| 54:1:230:G:O2'    | 54:1:231:A:H5'    | 2.10                     | 0.52              |
| 54:1:613:A:H2'    | 54:1:613:A:N3     | 2.23                     | 0.52              |
| 54:1:1681:G:H21   | 54:1:1762:A:H3'   | 1.74                     | 0.52              |
| 54:1:2004:G:H2'   | 54:1:2005:A:O4'   | 2.10                     | 0.52              |
| 54:1:2016:U:H2'   | 54:1:2017:U:C6    | 2.44                     | 0.52              |
| 59:8:68:THR:O     | 59:8:86:ILE:N     | 2.42                     | 0.52              |
| 59:8:424:THR:O    | 59:8:426:ALA:N    | 2.42                     | 0.52              |
| 59:8:425:LYS:C    | 59:8:428:GLN:H    | 2.18                     | 0.52              |
| 7:h:6:GLN:HA      | 7:h:9:GLN:HG2     | 1.92                     | 0.52              |
| 11:l:93:ASN:HA    | 11:l:96:LYS:HG3   | 1.91                     | 0.52              |
| 32:G:49:PHE:HA    | 32:G:52:ALA:HB3   | 1.91                     | 0.52              |
| 32:G:221:ARG:HB2  | 32:G:221:ARG:HH11 | 1.75                     | 0.52              |
| 35:J:133:ILE:H    | 35:J:133:ILE:CD1  | 2.19                     | 0.52              |
| 40:O:39:PRO:HB2   | 53:3:1123:U:O4    | 2.09                     | 0.52              |
| 42:Q:7:VAL:HG13   | 47:V:30:HIS:CD2   | 2.45                     | 0.52              |
| 49:X:36:ARG:HG2   | 53:3:1320:C:C4    | 2.45                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:225:C:C2'    | 53:3:226:G:H5''   | 2.38                     | 0.52              |
| 53:3:558:G:H2'    | 53:3:559:A:H2     | 1.74                     | 0.52              |
| 53:3:945:G:C6     | 53:3:946:A:C8     | 2.98                     | 0.52              |
| 53:3:1059:C:H2'   | 53:3:1060:U:H6    | 1.74                     | 0.52              |
| 53:3:1511:G:H2'   | 53:3:1512:U:O4'   | 2.10                     | 0.52              |
| 54:1:129:C:H2'    | 54:1:130:C:C6     | 2.45                     | 0.52              |
| 54:1:563:A:H2'    | 54:1:564:C:C6     | 2.44                     | 0.52              |
| 54:1:665:U:H2'    | 54:1:666:A:C8     | 2.45                     | 0.52              |
| 54:1:2163:A:N3    | 54:1:2163:A:H2'   | 2.25                     | 0.52              |
| 54:1:2277:G:H3'   | 54:1:2278:A:H5''  | 1.92                     | 0.52              |
| 59:8:111:MET:HE3  | 59:8:137:ARG:HD3  | 1.91                     | 0.52              |
| 59:8:363:ILE:HG21 | 59:8:377:VAL:HG22 | 1.91                     | 0.52              |
| 5:f:23:ILE:HD11   | 5:f:42:VAL:HG11   | 1.91                     | 0.52              |
| 5:f:89:VAL:HG21   | 5:f:162:ARG:HE    | 1.73                     | 0.52              |
| 9:j:49:ASP:OD1    | 9:j:118:MET:HB3   | 2.09                     | 0.52              |
| 16:q:69:ARG:HH22  | 16:q:74:SER:CA    | 2.18                     | 0.52              |
| 21:v:80:HIS:HB3   | 21:v:83:LYS:O     | 2.10                     | 0.52              |
| 24:y:48:ARG:HB3   | 24:y:52:ARG:HH22  | 1.74                     | 0.52              |
| 44:S:48:GLN:HB2   | 49:X:12:LEU:CD1   | 2.40                     | 0.52              |
| 53:3:16:A:H2'     | 53:3:16:A:N3      | 2.24                     | 0.52              |
| 53:3:722:G:C8     | 53:3:724:G:H1'    | 2.44                     | 0.52              |
| 54:1:974:G:H1'    | 54:1:975:A:C8     | 2.44                     | 0.52              |
| 54:1:1440:U:H2'   | 54:1:1441:G:C8    | 2.45                     | 0.52              |
| 54:1:2323:G:O2'   | 54:1:2324:U:H5'   | 2.10                     | 0.52              |
| 54:1:2533:U:C2'   | 54:1:2534:A:H5'   | 2.40                     | 0.52              |
| 59:8:354:LYS:HD2  | 59:8:354:LYS:O    | 2.09                     | 0.52              |
| 2:c:175:LEU:HD22  | 2:c:190:LYS:O     | 2.10                     | 0.52              |
| 3:d:138:LEU:O     | 3:d:142:ALA:N     | 2.43                     | 0.52              |
| 10:k:13:ASN:ND2   | 10:k:98:ARG:N     | 2.57                     | 0.52              |
| 22:w:49:CYS:SG    | 22:w:53:HIS:HA    | 2.50                     | 0.52              |
| 32:G:35:ASN:O     | 32:G:36:LYS:HB2   | 2.10                     | 0.52              |
| 34:I:21:LYS:HD2   | 53:3:430:A:OP2    | 2.10                     | 0.52              |
| 35:J:96:GLN:HE21  | 35:J:123:LEU:HG   | 1.74                     | 0.52              |
| 41:P:13:LYS:HD3   | 41:P:13:LYS:N     | 2.24                     | 0.52              |
| 42:Q:63:THR:HG23  | 42:Q:92:VAL:HA    | 1.92                     | 0.52              |
| 44:S:48:GLN:OE1   | 44:S:48:GLN:N     | 2.43                     | 0.52              |
| 53:3:871:U:H5''   | 53:3:872:A:OP2    | 2.10                     | 0.52              |
| 53:3:1121:U:OP2   | 53:3:1121:U:H6    | 1.93                     | 0.52              |
| 53:3:1158:C:C5    | 53:3:1160:G:H1'   | 2.45                     | 0.52              |
| 53:3:1387:G:H2'   | 53:3:1388:C:C6    | 2.45                     | 0.52              |
| 54:1:215:G:C4'    | 54:1:216:A:H4'    | 2.40                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:351:C:H2'    | 54:1:352:A:H8     | 1.75                     | 0.52              |
| 54:1:812:C:O2'    | 54:1:813:U:H5'    | 2.09                     | 0.52              |
| 54:1:1857:G:H1'   | 54:1:1885:A:N6    | 2.25                     | 0.52              |
| 54:1:2070:A:H2'   | 54:1:2071:A:H8    | 1.73                     | 0.52              |
| 54:1:2805:C:H2'   | 54:1:2806:C:C6    | 2.44                     | 0.52              |
| 59:8:74:GLY:H     | 59:8:80:GLU:CG    | 2.23                     | 0.52              |
| 1:b:231:HIS:HA    | 1:b:241:LYS:HE3   | 1.92                     | 0.52              |
| 4:e:140:ILE:HD12  | 4:e:140:ILE:H     | 1.74                     | 0.52              |
| 8:i:20:SER:CB     | 8:i:21:PRO:HD3    | 2.35                     | 0.52              |
| 14:o:57:ALA:HA    | 14:o:60:GLU:OE1   | 2.11                     | 0.52              |
| 22:w:51:ARG:HG2   | 54:1:2365:G:P     | 2.49                     | 0.52              |
| 31:F:17:VAL:HG12  | 31:F:19:ARG:HG3   | 1.90                     | 0.52              |
| 32:G:72:LYS:NZ    | 32:G:74:ALA:HB3   | 2.25                     | 0.52              |
| 32:G:221:ARG:HH11 | 32:G:221:ARG:CB   | 2.24                     | 0.52              |
| 33:H:58:ARG:NH1   | 33:H:58:ARG:HB2   | 2.25                     | 0.52              |
| 34:I:183:ARG:H    | 34:I:183:ARG:HD3  | 1.75                     | 0.52              |
| 39:N:104:THR:HG23 | 53:3:1180:A:H5'   | 1.91                     | 0.52              |
| 43:R:3:ILE:HG22   | 43:R:4:ALA:N      | 2.25                     | 0.52              |
| 45:T:86:LEU:N     | 45:T:86:LEU:HD23  | 2.25                     | 0.52              |
| 53:3:815:A:H4'    | 53:3:817:C:C5     | 2.45                     | 0.52              |
| 53:3:936:C:H1'    | 53:3:1383:C:N4    | 2.25                     | 0.52              |
| 53:3:1065:U:H5''  | 53:3:1190:G:N1    | 2.23                     | 0.52              |
| 54:1:129:C:H2'    | 54:1:130:C:H6     | 1.75                     | 0.52              |
| 54:1:1808:A:H3'   | 54:1:1809:A:C8    | 2.45                     | 0.52              |
| 54:1:2373:G:H2'   | 54:1:2374:C:C6    | 2.45                     | 0.52              |
| 54:1:2677:G:H2'   | 54:1:2678:C:H6    | 1.75                     | 0.52              |
| 54:1:2679:A:H2'   | 54:1:2680:U:H6    | 1.73                     | 0.52              |
| 56:5:16:C:H5'     | 56:5:59:A:N1      | 2.24                     | 0.52              |
| 1:b:204:LEU:HD11  | 1:b:213:ARG:HH21  | 1.75                     | 0.51              |
| 2:c:152:PRO:HG2   | 2:c:153:GLY:H     | 1.74                     | 0.51              |
| 3:d:131:THR:HG23  | 54:1:321:U:H5''   | 1.92                     | 0.51              |
| 5:f:35:THR:C      | 5:f:36:LEU:HD22   | 2.35                     | 0.51              |
| 13:n:78:LYS:HG3   | 13:n:82:GLU:CD    | 2.34                     | 0.51              |
| 24:y:18:LEU:O     | 24:y:22:LEU:HB2   | 2.11                     | 0.51              |
| 26:A:17:SER:OG    | 26:A:35:ASP:HA    | 2.09                     | 0.51              |
| 32:G:16:GLY:HA3   | 32:G:39:ILE:HA    | 1.91                     | 0.51              |
| 33:H:111:ASP:O    | 33:H:115:VAL:HG23 | 2.10                     | 0.51              |
| 33:H:166:TRP:CZ2  | 53:3:1192:C:H4'   | 2.45                     | 0.51              |
| 46:U:67:ILE:HD12  | 46:U:67:ILE:N     | 2.24                     | 0.51              |
| 53:3:79:G:O2'     | 53:3:80:A:H5'     | 2.10                     | 0.51              |
| 53:3:389:A:H3'    | 53:3:390:U:H6     | 1.74                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:813:U:H2'    | 54:1:814:C:C6     | 2.42                     | 0.51              |
| 54:1:1152:C:H2'   | 54:1:1153:C:C6    | 2.46                     | 0.51              |
| 54:1:1909:C:H2'   | 54:1:1910:G:H8    | 1.75                     | 0.51              |
| 54:1:2493:U:C2'   | 54:1:2494:G:H5''  | 2.40                     | 0.51              |
| 54:1:2715:C:H2'   | 54:1:2716:C:O4'   | 2.10                     | 0.51              |
| 59:8:141:VAL:HG12 | 59:8:265:THR:O    | 2.10                     | 0.51              |
| 4:e:16:MET:HE1    | 4:e:27:VAL:HB     | 1.93                     | 0.51              |
| 4:e:166:ARG:NH1   | 4:e:166:ARG:HB2   | 2.25                     | 0.51              |
| 9:j:32:LEU:C      | 9:j:36:LEU:HD23   | 2.35                     | 0.51              |
| 14:o:106:LEU:C    | 14:o:106:LEU:HD23 | 2.34                     | 0.51              |
| 15:p:15:ASP:O     | 15:p:17:PRO:HD3   | 2.10                     | 0.51              |
| 18:s:3:THR:HG21   | 18:s:54:ALA:O     | 2.10                     | 0.51              |
| 21:v:46:LYS:O     | 21:v:50:MET:HG2   | 2.10                     | 0.51              |
| 29:D:35:ARG:CB    | 29:D:35:ARG:HH11  | 2.23                     | 0.51              |
| 32:G:15:PHE:O     | 32:G:40:ILE:HB    | 2.11                     | 0.51              |
| 33:H:69:THR:HG21  | 33:H:75:VAL:HG21  | 1.91                     | 0.51              |
| 35:J:17:VAL:HG21  | 35:J:55:VAL:HG12  | 1.91                     | 0.51              |
| 35:J:75:LEU:O     | 35:J:75:LEU:HD12  | 2.09                     | 0.51              |
| 36:K:38:ARG:NE    | 36:K:38:ARG:HA    | 2.25                     | 0.51              |
| 40:O:52:LEU:HA    | 40:O:62:ARG:HG2   | 1.92                     | 0.51              |
| 40:O:102:LEU:HD12 | 40:O:102:LEU:H    | 1.75                     | 0.51              |
| 42:Q:23:LEU:CD1   | 42:Q:58:ASN:HD22  | 2.22                     | 0.51              |
| 53:3:82:G:H2'     | 53:3:83:C:O4'     | 2.10                     | 0.51              |
| 53:3:1259:C:H3'   | 53:3:1260:G:C5'   | 2.30                     | 0.51              |
| 54:1:465:G:H2'    | 54:1:466:A:C8     | 2.46                     | 0.51              |
| 54:1:1420:A:H5'   | 54:1:1421:G:OP2   | 2.10                     | 0.51              |
| 54:1:2808:G:H5'   | 54:1:2809:A:OP1   | 2.11                     | 0.51              |
| 1:b:206:LYS:HB2   | 54:1:729:G:N7     | 2.25                     | 0.51              |
| 2:c:11:MET:O      | 54:1:2682:A:H5'   | 2.10                     | 0.51              |
| 2:c:202:ILE:HD12  | 2:c:202:ILE:N     | 2.24                     | 0.51              |
| 7:h:3:LEU:HG      | 7:h:4:ASN:N       | 2.25                     | 0.51              |
| 15:p:51:ASN:O     | 54:1:2845:U:H5''  | 2.10                     | 0.51              |
| 20:u:12:VAL:HG23  | 20:u:20:LYS:O     | 2.09                     | 0.51              |
| 22:w:10:ARG:HD2   | 54:1:2280:G:O6    | 2.10                     | 0.51              |
| 38:M:9:MET:CA     | 38:M:26:MET:HE1   | 2.39                     | 0.51              |
| 41:P:106:ILE:O    | 41:P:106:ILE:HG13 | 2.10                     | 0.51              |
| 53:3:977:A:H5''   | 53:3:977:A:N3     | 2.26                     | 0.51              |
| 54:1:322:A:H5'    | 54:1:340:A:H1'    | 1.92                     | 0.51              |
| 54:1:578:G:H21    | 54:1:1252:G:N2    | 2.09                     | 0.51              |
| 54:1:2047:C:H2'   | 54:1:2048:G:H8    | 1.75                     | 0.51              |
| 54:1:2086:U:H2'   | 54:1:2087:G:C8    | 2.45                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:2741:A:H2'   | 54:1:2742:G:O4'   | 2.10                     | 0.51              |
| 54:1:2834:G:H2'   | 54:1:2879:A:N6    | 2.25                     | 0.51              |
| 55:2:119:A:C2     | 55:2:120:A:C1'    | 2.91                     | 0.51              |
| 59:8:74:GLY:HA3   | 59:8:79:TYR:CD2   | 2.45                     | 0.51              |
| 59:8:83:ARG:C     | 59:8:84:ILE:HD12  | 2.36                     | 0.51              |
| 59:8:85:ASN:HB3   | 59:8:382:ILE:HD11 | 1.91                     | 0.51              |
| 1:b:191:LEU:HD23  | 1:b:192:GLY:N     | 2.24                     | 0.51              |
| 21:v:42:LEU:C     | 21:v:42:LEU:HD12  | 2.36                     | 0.51              |
| 22:w:42:HIS:HB3   | 22:w:75:PHE:CE1   | 2.46                     | 0.51              |
| 26:A:49:ARG:HH12  | 49:X:45:GLY:HA3   | 1.74                     | 0.51              |
| 33:H:177:LEU:HD23 | 53:3:1112:C:H42   | 1.75                     | 0.51              |
| 37:L:27:ASN:HA    | 37:L:30:MET:HB2   | 1.92                     | 0.51              |
| 40:O:20:GLN:O     | 40:O:24:GLU:HG3   | 2.11                     | 0.51              |
| 52:a:200:LYS:HD2  | 52:a:201:PRO:HD2  | 1.92                     | 0.51              |
| 53:3:403:C:H2'    | 53:3:404:G:O4'    | 2.10                     | 0.51              |
| 53:3:483:C:H2'    | 53:3:484:G:C8     | 2.45                     | 0.51              |
| 53:3:802:A:H2'    | 53:3:803:G:O4'    | 2.09                     | 0.51              |
| 53:3:908:A:H2'    | 53:3:909:A:C8     | 2.44                     | 0.51              |
| 53:3:1202:U:H2'   | 53:3:1203:C:O4'   | 2.10                     | 0.51              |
| 54:1:657:U:H2'    | 54:1:658:U:C6     | 2.46                     | 0.51              |
| 54:1:861:A:H2'    | 54:1:862:G:O4'    | 2.10                     | 0.51              |
| 54:1:2423:U:O2'   | 54:1:2425:A:H2'   | 2.10                     | 0.51              |
| 54:1:2533:U:H2'   | 54:1:2534:A:H5'   | 1.92                     | 0.51              |
| 59:8:99:VAL:HG13  | 59:8:103:MET:HE2  | 1.92                     | 0.51              |
| 3:d:40:ARG:HE     | 3:d:92:HIS:CD2    | 2.29                     | 0.51              |
| 5:f:136:ASP:HB3   | 5:f:139:VAL:HB    | 1.91                     | 0.51              |
| 6:g:134:VAL:HG23  | 6:g:135:HIS:H     | 1.75                     | 0.51              |
| 9:j:84:ILE:HG23   | 9:j:84:ILE:O      | 2.10                     | 0.51              |
| 9:j:140:LEU:HG    | 9:j:142:ILE:HG22  | 1.91                     | 0.51              |
| 11:l:101:ILE:HG13 | 11:l:102:GLY:N    | 2.25                     | 0.51              |
| 13:n:35:LYS:NZ    | 13:n:110:MET:HG2  | 2.25                     | 0.51              |
| 16:q:106:THR:O    | 16:q:110:GLU:HG2  | 2.10                     | 0.51              |
| 17:r:22:LEU:CD1   | 17:r:94:THR:HB    | 2.36                     | 0.51              |
| 17:r:76:LYS:HB2   | 17:r:85:LYS:HB3   | 1.93                     | 0.51              |
| 23:x:12:VAL:HG22  | 23:x:28:PHE:HB2   | 1.93                     | 0.51              |
| 40:O:39:PRO:HB3   | 53:3:1123:U:O4    | 2.10                     | 0.51              |
| 42:Q:113:ARG:HH22 | 53:3:501:C:P      | 2.33                     | 0.51              |
| 44:S:25:GLU:HG2   | 44:S:26:LEU:HD12  | 1.93                     | 0.51              |
| 48:W:34:GLU:HB3   | 51:Z:18:PHE:CZ    | 2.45                     | 0.51              |
| 53:3:313:A:H2'    | 53:3:314:C:H6     | 1.76                     | 0.51              |
| 53:3:920:U:C2     | 53:3:1080:A:C5    | 2.98                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 54:1:11:C:H2'    | 54:1:12:U:H5''   | 1.91                     | 0.51              |
| 54:1:23:G:H2'    | 54:1:24:G:H8     | 1.76                     | 0.51              |
| 54:1:1922:G:H2'  | 54:1:1923:U:C6   | 2.46                     | 0.51              |
| 54:1:2055:C:H5'  | 54:1:2056:G:O5'  | 2.11                     | 0.51              |
| 54:1:2593:U:H2'  | 54:1:2594:C:C6   | 2.45                     | 0.51              |
| 54:1:2662:A:H2'  | 54:1:2663:G:O4'  | 2.10                     | 0.51              |
| 59:8:13:ILE:HG22 | 59:8:108:GLY:CA  | 2.33                     | 0.51              |
| 13:n:78:LYS:HE3  | 13:n:82:GLU:OE2  | 2.10                     | 0.51              |
| 15:p:51:ASN:O    | 15:p:52:ARG:HD3  | 2.09                     | 0.51              |
| 18:s:57:ASN:OD1  | 54:1:495:G:H1'   | 2.10                     | 0.51              |
| 21:v:26:PHE:CE1  | 21:v:42:LEU:HD11 | 2.46                     | 0.51              |
| 22:w:17:LEU:HD21 | 22:w:37:ARG:NH2  | 2.26                     | 0.51              |
| 26:A:6:HIS:HB3   | 26:A:7:PRO:HD2   | 1.93                     | 0.51              |
| 32:G:31:PHE:O    | 32:G:39:ILE:N    | 2.43                     | 0.51              |
| 35:J:45:VAL:O    | 35:J:71:ILE:N    | 2.44                     | 0.51              |
| 36:K:73:GLU:HA   | 36:K:76:THR:HG23 | 1.93                     | 0.51              |
| 37:L:25:PHE:CD1  | 37:L:100:MET:HB3 | 2.46                     | 0.51              |
| 40:O:73:LEU:O    | 53:3:1123:U:C2'  | 2.59                     | 0.51              |
| 44:S:58:ARG:HH21 | 53:3:980:C:C4'   | 2.24                     | 0.51              |
| 47:V:11:VAL:HG11 | 47:V:20:ILE:HD11 | 1.93                     | 0.51              |
| 50:Y:43:LYS:HB3  | 50:Y:85:LEU:CD2  | 2.40                     | 0.51              |
| 53:3:603:U:H2'   | 53:3:604:G:H8    | 1.76                     | 0.51              |
| 53:3:1256:A:H1'  | 53:3:1258:G:C5   | 2.46                     | 0.51              |
| 54:1:1139:G:H2'  | 54:1:1140:C:H6   | 1.75                     | 0.51              |
| 54:1:1387:A:H2'  | 54:1:1388:G:H8   | 1.76                     | 0.51              |
| 54:1:2049:G:O2'  | 54:1:2050:C:H5'  | 2.11                     | 0.51              |
| 54:1:2267:A:H5'' | 54:1:2268:A:H5'  | 1.93                     | 0.51              |
| 54:1:2698:U:H2'  | 54:1:2699:C:C6   | 2.46                     | 0.51              |
| 55:2:30:C:H1'    | 55:2:57:A:H61    | 1.75                     | 0.51              |
| 59:8:17:ALA:C    | 59:8:23:LYS:HZ2  | 2.19                     | 0.51              |
| 20:u:58:VAL:HG11 | 20:u:60:LYS:HZ3  | 1.75                     | 0.51              |
| 35:J:14:LEU:C    | 35:J:14:LEU:HD23 | 2.35                     | 0.51              |
| 35:J:96:GLN:NE2  | 35:J:98:ALA:HB2  | 2.25                     | 0.51              |
| 41:P:30:ILE:CB   | 41:P:45:THR:HG22 | 2.37                     | 0.51              |
| 45:T:80:LEU:HA   | 45:T:83:ARG:CD   | 2.40                     | 0.51              |
| 45:T:80:LEU:O    | 45:T:83:ARG:HG2  | 2.10                     | 0.51              |
| 53:3:31:G:N2     | 53:3:47:C:H5''   | 2.23                     | 0.51              |
| 53:3:407:U:H2'   | 53:3:408:A:H8    | 1.74                     | 0.51              |
| 53:3:411:A:C4    | 53:3:413:G:H1'   | 2.46                     | 0.51              |
| 53:3:458:U:H2'   | 53:3:459:A:C8    | 2.46                     | 0.51              |
| 53:3:1092:A:H2'  | 53:3:1092:A:N3   | 2.26                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:3:1143:G:H2'  | 53:3:1144:G:C8   | 2.46                     | 0.51              |
| 54:1:473:G:O2'   | 54:1:474:G:H5'   | 2.09                     | 0.51              |
| 54:1:644:A:H61   | 54:1:2349:G:H21  | 1.59                     | 0.51              |
| 54:1:945:A:C5    | 54:1:2448:A:C2   | 2.98                     | 0.51              |
| 54:1:1528:A:H2'  | 54:1:1529:G:O4'  | 2.10                     | 0.51              |
| 54:1:1550:C:H2'  | 54:1:1551:A:C8   | 2.46                     | 0.51              |
| 54:1:1770:G:O2'  | 54:1:1771:C:H5'  | 2.11                     | 0.51              |
| 54:1:1827:U:O2'  | 54:1:1828:G:H5'  | 2.11                     | 0.51              |
| 54:1:1936:A:H2   | 54:1:1943:U:N3   | 1.97                     | 0.51              |
| 54:1:2273:A:H2'  | 54:1:2274:A:C8   | 2.46                     | 0.51              |
| 12:m:4:PRO:HG3   | 12:m:68:PHE:HE2  | 1.74                     | 0.51              |
| 13:n:55:ALA:HA   | 13:n:80:PHE:CE1  | 2.46                     | 0.51              |
| 23:x:66:VAL:HG23 | 23:x:67:LEU:HD12 | 1.92                     | 0.51              |
| 42:Q:32:VAL:CB   | 42:Q:55:ARG:HB3  | 2.39                     | 0.51              |
| 42:Q:86:VAL:HG23 | 42:Q:88:ASP:H    | 1.75                     | 0.51              |
| 42:Q:113:ARG:HB2 | 42:Q:118:VAL:HB  | 1.93                     | 0.51              |
| 43:R:77:LYS:HA   | 43:R:80:MET:HB2  | 1.91                     | 0.51              |
| 51:Z:16:ARG:HD2  | 51:Z:19:LYS:HD2  | 1.92                     | 0.51              |
| 53:3:596:A:H5'   | 53:3:596:A:H8    | 1.76                     | 0.51              |
| 53:3:779:C:H2'   | 53:3:780:A:O4'   | 2.11                     | 0.51              |
| 53:3:918:A:H2'   | 53:3:919:A:C8    | 2.46                     | 0.51              |
| 54:1:1387:A:H2'  | 54:1:1388:G:C8   | 2.46                     | 0.51              |
| 54:1:1853:A:H2'  | 54:1:1854:A:C8   | 2.45                     | 0.51              |
| 54:1:2121:G:O2'  | 54:1:2122:U:H5'  | 2.11                     | 0.51              |
| 54:1:2128:G:O2'  | 54:1:2174:C:H5'  | 2.10                     | 0.51              |
| 54:1:2405:G:H2'  | 54:1:2411:A:H62  | 1.76                     | 0.51              |
| 54:1:2677:G:H2'  | 54:1:2678:C:C6   | 2.46                     | 0.51              |
| 54:1:2710:C:H2'  | 54:1:2711:A:C8   | 2.46                     | 0.51              |
| 59:8:53:MET:HE1  | 59:8:63:ILE:CD1  | 2.37                     | 0.51              |
| 59:8:68:THR:HG22 | 59:8:69:THR:N    | 2.26                     | 0.51              |
| 3:d:145:ASP:CB   | 3:d:184:ASP:H    | 2.23                     | 0.51              |
| 4:e:67:THR:OG1   | 4:e:84:ILE:HG23  | 2.11                     | 0.51              |
| 5:f:14:VAL:HG13  | 5:f:25:ILE:HG23  | 1.93                     | 0.51              |
| 7:h:37:LYS:O     | 7:h:41:LEU:HB2   | 2.11                     | 0.51              |
| 7:h:58:THR:OG1   | 7:h:82:ILE:HB    | 2.11                     | 0.51              |
| 8:i:19:PRO:HB2   | 8:i:23:VAL:CG2   | 2.41                     | 0.51              |
| 11:l:8:PRO:HD3   | 54:1:1244:A:C5'  | 2.40                     | 0.51              |
| 12:m:136:MET:CE  | 21:v:77:VAL:HG12 | 2.41                     | 0.51              |
| 15:p:20:ARG:HD3  | 15:p:112:ARG:NH1 | 2.26                     | 0.51              |
| 21:v:38:LEU:HG   | 21:v:40:ILE:HD11 | 1.92                     | 0.51              |
| 24:y:17:GLU:O    | 24:y:20:ASN:HB2  | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 26:A:64:PHE:CD1  | 53:3:1011:C:H5'  | 2.45                     | 0.51              |
| 33:H:87:ARG:HH11 | 33:H:87:ARG:CB   | 2.23                     | 0.51              |
| 41:P:74:LYS:HE2  | 41:P:74:LYS:CA   | 2.41                     | 0.51              |
| 43:R:7:ASN:ND2   | 43:R:9:PRO:HD3   | 2.26                     | 0.51              |
| 43:R:96:VAL:H    | 53:3:1307:U:C2'  | 2.24                     | 0.51              |
| 44:S:19:TYR:O    | 44:S:21:ALA:N    | 2.43                     | 0.51              |
| 45:T:88:ARG:HD3  | 45:T:88:ARG:N    | 2.26                     | 0.51              |
| 52:a:172:HIS:HB3 | 54:1:2123:G:C4'  | 2.41                     | 0.51              |
| 53:3:355:C:H2'   | 53:3:356:A:O4'   | 2.10                     | 0.51              |
| 53:3:1166:G:OP2  | 53:3:1166:G:H8   | 1.94                     | 0.51              |
| 54:1:123:G:O2'   | 54:1:124:G:H5'   | 2.10                     | 0.51              |
| 54:1:1746:A:H2'  | 54:1:1747:U:H6   | 1.76                     | 0.51              |
| 54:1:2786:U:O2'  | 54:1:2787:C:H5'  | 2.11                     | 0.51              |
| 57:6:72:A:H2'    | 57:6:73:A:O4'    | 2.11                     | 0.51              |
| 59:8:605:PHE:O   | 59:8:610:PRO:HD3 | 2.11                     | 0.51              |
| 1:b:89:ASN:CG    | 1:b:196:ASN:HD21 | 2.19                     | 0.51              |
| 5:f:162:ARG:HD2  | 5:f:168:VAL:HG21 | 1.93                     | 0.51              |
| 18:s:88:ARG:HG3  | 18:s:94:ASP:OD2  | 2.11                     | 0.51              |
| 20:u:76:THR:HB   | 20:u:78:LYS:HE3  | 1.93                     | 0.51              |
| 27:B:2:VAL:HG22  | 54:1:2015:A:C2   | 2.46                     | 0.51              |
| 32:G:124:THR:HA  | 32:G:127:LYS:HG3 | 1.91                     | 0.51              |
| 35:J:96:GLN:HB2  | 35:J:97:PRO:HD2  | 1.92                     | 0.51              |
| 36:K:77:THR:HA   | 36:K:80:PHE:HB2  | 1.93                     | 0.51              |
| 37:L:101:ARG:O   | 37:L:105:GLU:HG3 | 2.10                     | 0.51              |
| 41:P:30:ILE:HA   | 41:P:45:THR:HA   | 1.93                     | 0.51              |
| 45:T:88:ARG:HG2  | 54:1:714:U:H5    | 1.75                     | 0.51              |
| 50:Y:2:ASN:CG    | 50:Y:3:ILE:H     | 2.18                     | 0.51              |
| 53:3:354:G:H2'   | 53:3:355:C:H5'   | 1.93                     | 0.51              |
| 53:3:370:C:H2'   | 53:3:371:A:H8    | 1.76                     | 0.51              |
| 54:1:699:A:H2'   | 54:1:700:G:O4'   | 2.11                     | 0.51              |
| 54:1:1351:C:H2'  | 54:1:1352:U:O4'  | 2.11                     | 0.51              |
| 54:1:1386:C:H2'  | 54:1:1387:A:C8   | 2.46                     | 0.51              |
| 54:1:1910:G:O2'  | 54:1:1911:U:H5'  | 2.11                     | 0.51              |
| 59:8:15:ILE:CD1  | 59:8:86:ILE:HD11 | 2.41                     | 0.51              |
| 1:b:42:ARG:HD2   | 1:b:42:ARG:N     | 2.26                     | 0.50              |
| 17:r:2:TYR:HB2   | 17:r:14:VAL:O    | 2.10                     | 0.50              |
| 28:C:38:PHE:HA   | 28:C:45:HIS:HD2  | 1.76                     | 0.50              |
| 33:H:106:ARG:N   | 33:H:106:ARG:HD2 | 2.26                     | 0.50              |
| 43:R:7:ASN:HD21  | 43:R:9:PRO:HB3   | 1.76                     | 0.50              |
| 47:V:58:VAL:HG13 | 47:V:74:LEU:CD1  | 2.41                     | 0.50              |
| 50:Y:11:ILE:O    | 50:Y:15:LYS:HG3  | 2.10                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:3:29:U:O2'    | 53:3:30:U:H5'    | 2.12                     | 0.50              |
| 53:3:79:G:H2'    | 53:3:80:A:O4'    | 2.10                     | 0.50              |
| 53:3:1074:G:H2'  | 53:3:1075:U:C6   | 2.46                     | 0.50              |
| 54:1:357:C:H2'   | 54:1:358:U:C6    | 2.46                     | 0.50              |
| 54:1:1426:G:H1'  | 54:1:1572:A:N6   | 2.25                     | 0.50              |
| 54:1:1539:U:H2'  | 54:1:1540:G:C8   | 2.45                     | 0.50              |
| 54:1:2818:U:H4'  | 54:1:2837:A:H4'  | 1.93                     | 0.50              |
| 59:8:414:PRO:HB3 | 59:8:446:ARG:HD3 | 1.92                     | 0.50              |
| 4:e:134:GLN:HB3  | 4:e:149:ARG:O    | 2.11                     | 0.50              |
| 7:h:74:ASP:O     | 7:h:77:VAL:HG12  | 2.11                     | 0.50              |
| 9:j:32:LEU:O     | 9:j:36:LEU:HD23  | 2.12                     | 0.50              |
| 23:x:12:VAL:CG2  | 23:x:28:PHE:HB2  | 2.41                     | 0.50              |
| 33:H:71:ARG:O    | 33:H:75:VAL:HG23 | 2.11                     | 0.50              |
| 34:I:62:ARG:HG3  | 34:I:62:ARG:NH1  | 2.26                     | 0.50              |
| 46:U:19:VAL:HG22 | 46:U:36:VAL:CG1  | 2.41                     | 0.50              |
| 53:3:217:C:H2'   | 53:3:218:U:C6    | 2.46                     | 0.50              |
| 53:3:575:G:HO2'  | 53:3:821:G:H5'   | 1.77                     | 0.50              |
| 53:3:1268:G:H22  | 53:3:1312:G:H1'  | 1.75                     | 0.50              |
| 53:3:1406:U:H2'  | 53:3:1407:C:C6   | 2.46                     | 0.50              |
| 54:1:753:A:O2'   | 54:1:754:U:H5'   | 2.10                     | 0.50              |
| 54:1:1353:A:H2'  | 54:1:1354:A:H8   | 1.76                     | 0.50              |
| 54:1:2229:U:H2'  | 54:1:2230:G:C8   | 2.45                     | 0.50              |
| 54:1:2547:A:H1'  | 54:1:2566:A:C6   | 2.46                     | 0.50              |
| 54:1:2692:G:H2'  | 54:1:2693:G:C8   | 2.46                     | 0.50              |
| 54:1:2895:G:H2'  | 54:1:2896:C:H6   | 1.77                     | 0.50              |
| 55:2:13:G:N2     | 55:2:16:G:H1'    | 2.22                     | 0.50              |
| 55:2:55:U:O2'    | 55:2:56:G:H5'    | 2.11                     | 0.50              |
| 59:8:399:ASP:OD1 | 59:8:400:PRO:HD3 | 2.11                     | 0.50              |
| 3:d:79:ARG:HD2   | 54:1:1258:U:O4'  | 2.11                     | 0.50              |
| 4:e:107:VAL:HB   | 4:e:108:PRO:HD3  | 1.93                     | 0.50              |
| 7:h:5:LEU:O      | 7:h:8:LYS:HB2    | 2.10                     | 0.50              |
| 12:m:96:ILE:C    | 12:m:97:GLN:OE1  | 2.55                     | 0.50              |
| 20:u:46:LYS:HZ3  | 20:u:48:VAL:HA   | 1.76                     | 0.50              |
| 29:D:11:LYS:HE2  | 54:1:771:G:OP2   | 2.12                     | 0.50              |
| 33:H:32:LEU:HA   | 33:H:35:ASP:OD2  | 2.11                     | 0.50              |
| 37:L:70:PRO:HG2  | 37:L:95:ARG:HG3  | 1.93                     | 0.50              |
| 38:M:9:MET:HA    | 38:M:26:MET:CE   | 2.39                     | 0.50              |
| 39:N:28:VAL:C    | 39:N:29:ILE:HD12 | 2.36                     | 0.50              |
| 40:O:36:VAL:CG1  | 53:3:1123:U:H5'  | 2.42                     | 0.50              |
| 40:O:46:LYS:HG2  | 40:O:68:ARG:HB3  | 1.94                     | 0.50              |
| 41:P:112:VAL:HB  | 48:W:72:ARG:NH2  | 2.24                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 42:Q:81:ILE:CD1  | 42:Q:96:THR:HG22  | 2.42                     | 0.50              |
| 43:R:108:ARG:HD3 | 43:R:109:LYS:N    | 2.26                     | 0.50              |
| 49:X:52:ASN:HB3  | 49:X:74:ALA:HB1   | 1.93                     | 0.50              |
| 53:3:334:C:H2'   | 53:3:335:C:H6     | 1.76                     | 0.50              |
| 54:1:2328:A:H2'  | 54:1:2329:U:H6    | 1.74                     | 0.50              |
| 54:1:2455:G:H2'  | 54:1:2456:C:H6    | 1.76                     | 0.50              |
| 13:n:35:LYS:NZ   | 13:n:110:MET:HE3  | 2.26                     | 0.50              |
| 13:n:43:GLU:OE2  | 13:n:46:ARG:HD3   | 2.12                     | 0.50              |
| 15:p:50:ARG:NH1  | 15:p:52:ARG:HG3   | 2.26                     | 0.50              |
| 17:r:51:VAL:O    | 17:r:52:PRO:C     | 2.54                     | 0.50              |
| 35:J:108:GLY:C   | 35:J:110:MET:H    | 2.20                     | 0.50              |
| 36:K:35:LYS:HD2  | 36:K:65:GLU:OE1   | 2.11                     | 0.50              |
| 36:K:36:ILE:HA   | 36:K:64:VAL:HG23  | 1.93                     | 0.50              |
| 40:O:74:VAL:HA   | 53:3:1123:U:O2'   | 2.11                     | 0.50              |
| 43:R:54:THR:O    | 43:R:57:ASP:OD2   | 2.29                     | 0.50              |
| 43:R:57:ASP:OD2  | 43:R:58:GLU:N     | 2.44                     | 0.50              |
| 49:X:14:LEU:HD13 | 49:X:37:SER:HB3   | 1.93                     | 0.50              |
| 49:X:44:ILE:HA   | 49:X:61:VAL:HG12  | 1.93                     | 0.50              |
| 49:X:47:THR:HG22 | 49:X:60:PHE:CA    | 2.41                     | 0.50              |
| 53:3:684:U:H2'   | 53:3:685:G:O4'    | 2.12                     | 0.50              |
| 53:3:801:U:H2'   | 53:3:802:A:C8     | 2.46                     | 0.50              |
| 53:3:1219:A:H2'  | 53:3:1220:G:C8    | 2.47                     | 0.50              |
| 54:1:289:G:H2'   | 54:1:290:U:C6     | 2.46                     | 0.50              |
| 54:1:1560:G:H2'  | 54:1:1560:G:N3    | 2.27                     | 0.50              |
| 56:5:21:A:H62    | 56:5:47:U:H1'     | 1.76                     | 0.50              |
| 59:8:56:GLU:O    | 59:8:60:GLY:N     | 2.26                     | 0.50              |
| 14:o:17:LYS:NZ   | 54:1:2380:C:H5'   | 2.25                     | 0.50              |
| 21:v:29:ILE:O    | 21:v:91:PHE:HB2   | 2.12                     | 0.50              |
| 22:w:34:VAL:HG11 | 22:w:41:PHE:HD2   | 1.76                     | 0.50              |
| 34:I:28:ASP:CG   | 34:I:29:THR:H     | 2.20                     | 0.50              |
| 39:N:98:ARG:NH1  | 39:N:103:VAL:HG21 | 2.27                     | 0.50              |
| 43:R:85:TYR:HE1  | 43:R:89:ARG:HH21  | 1.58                     | 0.50              |
| 45:T:80:LEU:HA   | 45:T:83:ARG:HG2   | 1.93                     | 0.50              |
| 53:3:32:A:H2'    | 53:3:33:A:H8      | 1.74                     | 0.50              |
| 53:3:1113:C:H2'  | 53:3:1114:C:C6    | 2.46                     | 0.50              |
| 59:8:115:ALA:HB1 | 59:8:149:ALA:HB1  | 1.92                     | 0.50              |
| 2:c:135:GLY:O    | 54:1:2580:U:H5''  | 2.12                     | 0.50              |
| 5:f:13:GLY:HA3   | 5:f:28:LYS:NZ     | 2.25                     | 0.50              |
| 7:h:54:VAL:O     | 7:h:54:VAL:HG22   | 2.12                     | 0.50              |
| 17:r:48:LYS:HD2  | 17:r:48:LYS:C     | 2.37                     | 0.50              |
| 19:t:69:ARG:NH2  | 54:1:1334:G:H5''  | 2.27                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 20:u:23:LYS:HG3  | 20:u:36:GLU:OE1   | 2.12                     | 0.50              |
| 27:B:39:ARG:O    | 27:B:40:HIS:HB2   | 2.12                     | 0.50              |
| 32:G:60:ALA:CB   | 32:G:223:GLY:HA3  | 2.42                     | 0.50              |
| 33:H:83:VAL:O    | 33:H:87:ARG:HG3   | 2.11                     | 0.50              |
| 34:I:24:VAL:HA   | 34:I:160:LEU:HD22 | 1.93                     | 0.50              |
| 36:K:51:ILE:O    | 36:K:53:LYS:N     | 2.45                     | 0.50              |
| 51:Z:28:LEU:HD23 | 51:Z:28:LEU:O     | 2.11                     | 0.50              |
| 52:a:220:ALA:HA  | 54:1:2176:A:C5'   | 2.42                     | 0.50              |
| 53:3:61:G:H2'    | 53:3:62:U:O4'     | 2.12                     | 0.50              |
| 53:3:335:C:H2'   | 53:3:336:A:H8     | 1.77                     | 0.50              |
| 53:3:674:G:H2'   | 53:3:675:A:C8     | 2.46                     | 0.50              |
| 53:3:1169:A:O2'  | 53:3:1170:A:H5'   | 2.11                     | 0.50              |
| 54:1:162:U:H2'   | 54:1:163:C:H5'    | 1.94                     | 0.50              |
| 54:1:800:A:C2    | 54:1:802:A:H8     | 2.29                     | 0.50              |
| 54:1:934:U:H2'   | 54:1:935:C:C6     | 2.46                     | 0.50              |
| 54:1:2105:U:H2'  | 54:1:2106:U:O4'   | 2.11                     | 0.50              |
| 58:4:18:G:C6     | 58:4:19:C:C5      | 3.00                     | 0.50              |
| 59:8:235:GLU:OE2 | 59:8:236:LYS:HG2  | 2.11                     | 0.50              |
| 59:8:463:GLU:H   | 59:8:671:ARG:HH22 | 1.60                     | 0.50              |
| 1:b:30:ALA:HB3   | 1:b:31:PRO:HD3    | 1.94                     | 0.50              |
| 1:b:175:LEU:HD13 | 54:1:1799:G:C5    | 2.47                     | 0.50              |
| 4:e:63:LYS:N     | 26:A:6:HIS:ND1    | 2.51                     | 0.50              |
| 5:f:74:MET:O     | 5:f:78:VAL:HG22   | 2.12                     | 0.50              |
| 21:v:80:HIS:ND1  | 21:v:81:PRO:HD2   | 2.27                     | 0.50              |
| 36:K:42:TRP:HB2  | 36:K:59:TYR:HB2   | 1.94                     | 0.50              |
| 42:Q:85:ARG:NH2  | 42:Q:87:LYS:HA    | 2.26                     | 0.50              |
| 43:R:51:GLN:HA   | 43:R:54:THR:CG2   | 2.38                     | 0.50              |
| 43:R:104:ASN:HB2 | 53:3:948:C:OP2    | 2.10                     | 0.50              |
| 53:3:217:C:H2'   | 53:3:218:U:H6     | 1.75                     | 0.50              |
| 53:3:580:C:H2'   | 53:3:581:G:C8     | 2.47                     | 0.50              |
| 53:3:609:A:C2'   | 53:3:610:U:H5'    | 2.41                     | 0.50              |
| 53:3:1462:C:H2'  | 53:3:1463:U:H6    | 1.73                     | 0.50              |
| 53:3:1539:C:O2'  | 53:3:1540:U:H5'   | 2.12                     | 0.50              |
| 54:1:155:A:H2'   | 54:1:156:A:H8     | 1.76                     | 0.50              |
| 54:1:622:G:H2'   | 54:1:623:C:C6     | 2.47                     | 0.50              |
| 54:1:1000:A:H2'  | 54:1:1001:A:C8    | 2.45                     | 0.50              |
| 54:1:1111:A:H2'  | 54:1:1111:A:N3    | 2.26                     | 0.50              |
| 54:1:1405:U:H2'  | 54:1:1406:U:C6    | 2.47                     | 0.50              |
| 1:b:13:ARG:HH12  | 54:1:1977:A:H2    | 1.60                     | 0.50              |
| 1:b:90:ILE:HD12  | 1:b:102:TYR:CD1   | 2.47                     | 0.50              |
| 4:e:121:PHE:CE1  | 4:e:127:TYR:HB2   | 2.47                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:m:133:LYS:C    | 12:m:133:LYS:HD3  | 2.36                     | 0.50              |
| 18:s:83:LYS:HG3   | 18:s:97:LEU:CD2   | 2.42                     | 0.50              |
| 23:x:39:VAL:HG12  | 23:x:42:GLU:H     | 1.77                     | 0.50              |
| 35:J:24:VAL:HG13  | 35:J:24:VAL:O     | 2.12                     | 0.50              |
| 37:L:115:MET:HA   | 37:L:118:ARG:HB2  | 1.93                     | 0.50              |
| 40:O:43:PRO:HG3   | 53:3:1150:A:O2'   | 2.12                     | 0.50              |
| 40:O:80:THR:HB    | 40:O:83:THR:CG2   | 2.36                     | 0.50              |
| 52:a:165:ASN:CB   | 52:a:171:ILE:HG22 | 2.41                     | 0.50              |
| 53:3:893:C:H2'    | 53:3:894:G:H8     | 1.76                     | 0.50              |
| 53:3:1342:C:H2'   | 53:3:1343:G:C8    | 2.47                     | 0.50              |
| 53:3:1417:G:H2'   | 53:3:1482:G:N2    | 2.27                     | 0.50              |
| 53:3:1517:G:H2'   | 53:3:1518:A:C5'   | 2.42                     | 0.50              |
| 54:1:1075:C:H2'   | 54:1:1076:C:H5''  | 1.93                     | 0.50              |
| 54:1:1103:A:H5''  | 54:1:1104:C:H5    | 1.77                     | 0.50              |
| 54:1:1139:G:O2'   | 54:1:1140:C:H5'   | 2.12                     | 0.50              |
| 54:1:1710:G:H2'   | 54:1:1711:A:H8    | 1.76                     | 0.50              |
| 54:1:2134:A:C2    | 54:1:2158:A:H5'   | 2.47                     | 0.50              |
| 55:2:55:U:H2'     | 55:2:56:G:C8      | 2.46                     | 0.50              |
| 57:6:14:A:H2'     | 57:6:15:G:O4'     | 2.11                     | 0.50              |
| 59:8:624:PRO:HA   | 59:8:650:THR:O    | 2.12                     | 0.50              |
| 1:b:7:PRO:HB3     | 1:b:13:ARG:HG3    | 1.92                     | 0.50              |
| 3:d:138:LEU:HD22  | 3:d:146:VAL:HG11  | 1.94                     | 0.50              |
| 6:g:94:ILE:HG13   | 6:g:122:LEU:HB2   | 1.94                     | 0.50              |
| 16:q:91:ARG:HH11  | 54:1:997:G:H5''   | 1.76                     | 0.50              |
| 33:H:102:ILE:HG22 | 33:H:103:ALA:N    | 2.27                     | 0.50              |
| 33:H:123:LEU:HD21 | 33:H:129:PHE:CB   | 2.38                     | 0.50              |
| 39:N:122:ARG:HB2  | 53:3:1349:A:OP1   | 2.12                     | 0.50              |
| 42:Q:99:GLY:HA2   | 42:Q:103:CYS:O    | 2.11                     | 0.50              |
| 52:a:212:VAL:O    | 52:a:224:VAL:HG22 | 2.11                     | 0.50              |
| 53:3:41:G:O2'     | 53:3:42:G:H5'     | 2.12                     | 0.50              |
| 53:3:399:G:H2'    | 53:3:400:C:H6     | 1.76                     | 0.50              |
| 53:3:547:A:H4'    | 53:3:548:G:O5'    | 2.12                     | 0.50              |
| 53:3:756:C:H2'    | 53:3:757:U:O4'    | 2.12                     | 0.50              |
| 53:3:940:C:H2'    | 53:3:941:G:H8     | 1.76                     | 0.50              |
| 53:3:1352:C:H2'   | 53:3:1353:G:H8    | 1.76                     | 0.50              |
| 54:1:494:G:H2'    | 54:1:495:G:C8     | 2.47                     | 0.50              |
| 54:1:851:C:H2'    | 54:1:852:U:C6     | 2.47                     | 0.50              |
| 54:1:2372:U:H2'   | 54:1:2373:G:H8    | 1.76                     | 0.50              |
| 59:8:158:ILE:HG21 | 59:8:166:PRO:HB3  | 1.94                     | 0.50              |
| 1:b:184:GLU:OE2   | 54:1:2222:C:H4'   | 2.11                     | 0.49              |
| 2:c:122:VAL:HG11  | 2:c:141:ARG:NH1   | 2.26                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:e:71:LYS:HA    | 4:e:80:GLN:HE22  | 1.76                     | 0.49              |
| 5:f:147:LEU:HA   | 5:f:150:TYR:HD2  | 1.78                     | 0.49              |
| 13:n:47:VAL:O    | 13:n:50:PRO:HD2  | 2.12                     | 0.49              |
| 14:o:47:VAL:CG2  | 55:2:114:C:H4'   | 2.42                     | 0.49              |
| 15:p:88:ARG:NH1  | 15:p:113:LEU:HA  | 2.27                     | 0.49              |
| 34:I:23:GLY:HA3  | 53:3:409:U:OP1   | 2.11                     | 0.49              |
| 36:K:25:TYR:CD1  | 36:K:74:LEU:HD11 | 2.46                     | 0.49              |
| 37:L:62:GLU:O    | 37:L:66:GLU:N    | 2.45                     | 0.49              |
| 37:L:151:ALA:OXT | 53:3:1538:C:H5'  | 2.12                     | 0.49              |
| 43:R:26:LYS:C    | 43:R:26:LYS:HD3  | 2.37                     | 0.49              |
| 45:T:42:PHE:HB3  | 45:T:52:ARG:HH22 | 1.76                     | 0.49              |
| 53:3:37:U:O2'    | 53:3:38:G:H5'    | 2.12                     | 0.49              |
| 53:3:151:A:H2'   | 53:3:152:A:O4'   | 2.12                     | 0.49              |
| 53:3:689:C:H2'   | 53:3:690:G:C8    | 2.47                     | 0.49              |
| 53:3:1080:A:O5'  | 53:3:1081:A:H5'' | 2.12                     | 0.49              |
| 54:1:847:U:O2    | 54:1:847:U:H2'   | 2.10                     | 0.49              |
| 54:1:1326:U:H2'  | 54:1:1327:A:H8   | 1.76                     | 0.49              |
| 54:1:1823:G:O2'  | 54:1:1824:G:H5'  | 2.12                     | 0.49              |
| 54:1:2188:U:H2'  | 54:1:2189:U:C1'  | 2.41                     | 0.49              |
| 54:1:2626:C:H2'  | 54:1:2627:G:C8   | 2.46                     | 0.49              |
| 55:2:51:G:H2'    | 55:2:52:A:O4'    | 2.12                     | 0.49              |
| 1:b:180:MET:HB2  | 1:b:267:VAL:HB   | 1.94                     | 0.49              |
| 12:m:11:LYS:HG2  | 12:m:86:LYS:HD3  | 1.93                     | 0.49              |
| 32:G:18:GLN:O    | 32:G:19:THR:HB   | 2.12                     | 0.49              |
| 32:G:45:THR:HG23 | 32:G:200:PRO:HD2 | 1.94                     | 0.49              |
| 32:G:118:THR:HB  | 32:G:119:GLN:NE2 | 2.26                     | 0.49              |
| 34:I:101:VAL:HB  | 34:I:113:ALA:HB1 | 1.94                     | 0.49              |
| 36:K:74:LEU:HG   | 36:K:78:PHE:HE1  | 1.77                     | 0.49              |
| 38:M:76:ARG:HG2  | 38:M:76:ARG:HH11 | 1.78                     | 0.49              |
| 39:N:34:LEU:HD21 | 39:N:48:ARG:HH11 | 1.77                     | 0.49              |
| 43:R:95:PRO:HG2  | 43:R:101:THR:CG2 | 2.42                     | 0.49              |
| 46:U:14:ARG:NE   | 46:U:42:ILE:HD13 | 2.26                     | 0.49              |
| 53:3:436:C:H2'   | 53:3:437:U:C6    | 2.47                     | 0.49              |
| 53:3:590:U:H2'   | 53:3:591:U:H6    | 1.77                     | 0.49              |
| 53:3:1171:A:N6   | 53:3:1172:C:N3   | 2.60                     | 0.49              |
| 54:1:75:G:H22    | 54:1:111:A:H2    | 1.61                     | 0.49              |
| 54:1:208:C:H2'   | 54:1:209:C:H6    | 1.77                     | 0.49              |
| 54:1:759:G:H2'   | 54:1:760:G:H8    | 1.77                     | 0.49              |
| 54:1:871:U:H2'   | 54:1:872:U:C6    | 2.47                     | 0.49              |
| 54:1:1355:G:O2'  | 54:1:1356:G:H5'  | 2.12                     | 0.49              |
| 54:1:1487:U:H2'  | 54:1:1488:C:H6   | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:2163:A:H3'   | 54:1:2164:C:H5'   | 1.92                     | 0.49              |
| 54:1:2196:C:O2'   | 54:1:2197:U:H5'   | 2.12                     | 0.49              |
| 1:b:167:ASP:OD1   | 1:b:167:ASP:O     | 2.29                     | 0.49              |
| 1:b:257:ARG:HG2   | 1:b:257:ARG:HH11  | 1.77                     | 0.49              |
| 5:f:154:GLU:OE2   | 5:f:155:PRO:HD2   | 2.11                     | 0.49              |
| 12:m:47:GLU:O     | 12:m:51:ARG:HG3   | 2.12                     | 0.49              |
| 13:n:99:LYS:O     | 27:B:41:HIS:HA    | 2.12                     | 0.49              |
| 15:p:113:LEU:HD11 | 53:3:1441:A:N3    | 2.28                     | 0.49              |
| 33:H:120:THR:OG1  | 33:H:188:ALA:HB2  | 2.12                     | 0.49              |
| 33:H:129:PHE:O    | 33:H:133:MET:HG2  | 2.12                     | 0.49              |
| 34:I:103:ARG:HD2  | 34:I:169:TRP:HZ2  | 1.77                     | 0.49              |
| 45:T:74:VAL:O     | 45:T:78:THR:HG23  | 2.12                     | 0.49              |
| 51:Z:67:THR:C     | 53:3:1167:A:N7    | 2.71                     | 0.49              |
| 53:3:441:A:H2'    | 53:3:441:A:N3     | 2.26                     | 0.49              |
| 53:3:972:C:O2'    | 53:3:973:G:H5'    | 2.12                     | 0.49              |
| 53:3:1017:U:H2'   | 53:3:1018:G:H8    | 1.77                     | 0.49              |
| 53:3:1229:A:H2'   | 53:3:1230:C:C6    | 2.48                     | 0.49              |
| 54:1:118:A:OP2    | 54:1:119:A:H2'    | 2.13                     | 0.49              |
| 54:1:419:U:H2'    | 54:1:420:C:H6     | 1.76                     | 0.49              |
| 54:1:472:A:H2'    | 54:1:473:G:H5'    | 1.93                     | 0.49              |
| 54:1:1412:U:H2'   | 54:1:1413:A:C8    | 2.47                     | 0.49              |
| 54:1:2233:U:H2'   | 54:1:2234:G:H8    | 1.77                     | 0.49              |
| 54:1:2266:A:H4'   | 54:1:2267:A:N3    | 2.28                     | 0.49              |
| 54:1:2364:C:H2'   | 54:1:2365:G:O4'   | 2.12                     | 0.49              |
| 54:1:2404:U:H2'   | 54:1:2405:G:O4'   | 2.13                     | 0.49              |
| 59:8:11:ARG:HG3   | 59:8:11:ARG:HH11  | 1.77                     | 0.49              |
| 59:8:99:VAL:CG1   | 59:8:103:MET:HE2  | 2.43                     | 0.49              |
| 59:8:100:GLU:CD   | 59:8:412:PRO:HG3  | 2.37                     | 0.49              |
| 59:8:315:GLU:CG   | 59:8:316:PRO:HD2  | 2.42                     | 0.49              |
| 59:8:492:GLU:HB2  | 59:8:571:VAL:HG22 | 1.94                     | 0.49              |
| 5:f:27:GLY:HA3    | 5:f:78:VAL:HB     | 1.94                     | 0.49              |
| 5:f:125:PRO:HG2   | 5:f:129:GLU:HG3   | 1.94                     | 0.49              |
| 6:g:45:GLU:HA     | 6:g:48:GLU:CG     | 2.41                     | 0.49              |
| 7:h:61:ARG:HB3    | 54:1:1046:A:H4'   | 1.95                     | 0.49              |
| 9:j:28:LEU:HD23   | 9:j:28:LEU:C      | 2.37                     | 0.49              |
| 10:k:58:LEU:N     | 10:k:58:LEU:HD23  | 2.27                     | 0.49              |
| 19:t:11:LEU:HD22  | 19:t:50:LEU:HD12  | 1.94                     | 0.49              |
| 24:y:45:GLN:O     | 24:y:49:ASP:N     | 2.44                     | 0.49              |
| 34:I:6:PRO:HG2    | 53:3:428:G:OP2    | 2.11                     | 0.49              |
| 36:K:53:LYS:HB2   | 36:K:54:LEU:HD23  | 1.94                     | 0.49              |
| 37:L:46:LEU:HD12  | 37:L:49:LEU:HD23  | 1.92                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:S:8:ARG:HH22   | 53:3:994:A:H1'    | 1.76                     | 0.49              |
| 52:a:54:LYS:HE3   | 52:a:205:LYS:CG   | 2.42                     | 0.49              |
| 53:3:966:G:C2'    | 53:3:967:C:H5'    | 2.38                     | 0.49              |
| 54:1:780:G:H2'    | 54:1:782:A:N7     | 2.27                     | 0.49              |
| 54:1:1487:U:H2'   | 54:1:1488:C:C6    | 2.47                     | 0.49              |
| 54:1:2637:U:H2'   | 54:1:2638:G:O4'   | 2.12                     | 0.49              |
| 59:8:159:LYS:HA   | 59:8:163:GLY:HA2  | 1.94                     | 0.49              |
| 59:8:301:ASP:O    | 59:8:303:LYS:N    | 2.45                     | 0.49              |
| 1:b:259:ASN:C     | 1:b:261:ARG:H     | 2.20                     | 0.49              |
| 4:e:130:GLY:HA2   | 4:e:152:ASP:HA    | 1.95                     | 0.49              |
| 5:f:16:VAL:HG11   | 5:f:49:LEU:HD11   | 1.95                     | 0.49              |
| 12:m:123:LYS:HE3  | 54:1:2483:C:N3    | 2.28                     | 0.49              |
| 22:w:34:VAL:HG11  | 22:w:41:PHE:CD2   | 2.48                     | 0.49              |
| 32:G:211:LEU:HD23 | 32:G:211:LEU:C    | 2.37                     | 0.49              |
| 38:M:6:ILE:O      | 38:M:9:MET:HB3    | 2.11                     | 0.49              |
| 38:M:32:LYS:HD3   | 38:M:35:ILE:HD11  | 1.95                     | 0.49              |
| 38:M:94:VAL:HG21  | 38:M:101:ALA:HB2  | 1.93                     | 0.49              |
| 41:P:123:PRO:HB2  | 41:P:125:LYS:HG2  | 1.95                     | 0.49              |
| 45:T:21:THR:HA    | 45:T:26:VAL:HG21  | 1.94                     | 0.49              |
| 53:3:334:C:H2'    | 53:3:335:C:C6     | 2.47                     | 0.49              |
| 53:3:825:A:H2'    | 53:3:826:C:C6     | 2.48                     | 0.49              |
| 53:3:948:C:H6     | 53:3:948:C:O5'    | 1.94                     | 0.49              |
| 53:3:1524:C:H2'   | 53:3:1525:G:H8    | 1.70                     | 0.49              |
| 54:1:3:U:H2'      | 54:1:4:U:H6       | 1.76                     | 0.49              |
| 54:1:503:A:H4'    | 54:1:505:A:H5''   | 1.93                     | 0.49              |
| 54:1:824:U:H2'    | 54:1:825:A:C8     | 2.48                     | 0.49              |
| 54:1:1683:U:H2'   | 54:1:1684:G:C8    | 2.47                     | 0.49              |
| 55:2:1:U:O4       | 55:2:2:G:C6       | 2.66                     | 0.49              |
| 59:8:253:ARG:O    | 59:8:256:VAL:HG22 | 2.12                     | 0.49              |
| 59:8:353:VAL:HG11 | 59:8:395:ASP:HB3  | 1.93                     | 0.49              |
| 1:b:79:ARG:NE     | 1:b:92:LEU:HD22   | 2.27                     | 0.49              |
| 3:d:112:LEU:HB3   | 3:d:118:LEU:HB2   | 1.95                     | 0.49              |
| 4:e:121:PHE:CZ    | 4:e:169:LEU:HD12  | 2.48                     | 0.49              |
| 7:h:54:VAL:HG13   | 54:1:1084:A:C5'   | 2.43                     | 0.49              |
| 10:k:102:PRO:HB3  | 10:k:121:GLU:HB2  | 1.94                     | 0.49              |
| 11:l:4:ASN:O      | 54:1:1243:C:H1'   | 2.13                     | 0.49              |
| 20:u:39:ASN:HD22  | 20:u:62:ALA:CB    | 2.15                     | 0.49              |
| 23:x:1:SER:HB2    | 54:1:1364:G:H3'   | 1.94                     | 0.49              |
| 32:G:125:PHE:CG   | 32:G:126:ASP:N    | 2.80                     | 0.49              |
| 32:G:129:THR:O    | 32:G:132:GLU:HG3  | 2.12                     | 0.49              |
| 34:I:90:LEU:O     | 34:I:94:GLU:HG2   | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:I:161:ALA:HA  | 34:I:164:ARG:NE  | 2.12                     | 0.49              |
| 35:J:22:LYS:HG3  | 53:3:1081:A:OP1  | 2.12                     | 0.49              |
| 37:L:125:ASP:HB2 | 37:L:131:GLY:H   | 1.77                     | 0.49              |
| 44:S:2:LYS:O     | 44:S:5:MET:N     | 2.45                     | 0.49              |
| 44:S:99:SER:CB   | 53:3:1187:G:H21  | 2.25                     | 0.49              |
| 52:a:5:THR:OG1   | 52:a:8:MET:HE3   | 2.13                     | 0.49              |
| 53:3:210:C:H4'   | 53:3:211:G:C2    | 2.46                     | 0.49              |
| 53:3:357:G:O2'   | 53:3:358:U:H5'   | 2.12                     | 0.49              |
| 53:3:676:A:H2'   | 53:3:677:U:H6    | 1.77                     | 0.49              |
| 53:3:678:U:H2'   | 53:3:679:C:H6    | 1.78                     | 0.49              |
| 53:3:818:G:H3'   | 53:3:819:A:H5'   | 1.93                     | 0.49              |
| 53:3:860:A:H2'   | 53:3:861:G:O4'   | 2.12                     | 0.49              |
| 53:3:1056:U:O4   | 53:3:1200:C:C2   | 2.66                     | 0.49              |
| 54:1:235:U:H2'   | 54:1:236:C:H6    | 1.76                     | 0.49              |
| 54:1:784:G:H5'   | 54:1:785:G:OP1   | 2.13                     | 0.49              |
| 54:1:1484:U:H2'  | 54:1:1485:U:H6   | 1.77                     | 0.49              |
| 54:1:1526:C:H2'  | 54:1:1527:G:O4'  | 2.12                     | 0.49              |
| 54:1:2393:U:H2'  | 54:1:2394:C:H6   | 1.77                     | 0.49              |
| 57:6:46:G:H2'    | 57:6:47:U:H5'    | 1.94                     | 0.49              |
| 13:n:90:ARG:HH11 | 54:1:2880:C:H4'  | 1.77                     | 0.49              |
| 16:q:30:VAL:HG21 | 54:1:580:U:O3'   | 2.13                     | 0.49              |
| 16:q:91:ARG:NH1  | 54:1:997:G:H5''  | 2.28                     | 0.49              |
| 22:w:42:HIS:HD2  | 22:w:73:ARG:HD3  | 1.75                     | 0.49              |
| 23:x:63:ILE:HG23 | 23:x:64:ASP:N    | 2.28                     | 0.49              |
| 25:z:8:GLN:HA    | 25:z:54:VAL:HG12 | 1.95                     | 0.49              |
| 34:I:34:GLU:HG2  | 34:I:34:GLU:O    | 2.12                     | 0.49              |
| 35:J:55:VAL:HG23 | 35:J:56:PRO:CD   | 2.42                     | 0.49              |
| 39:N:105:ARG:O   | 39:N:105:ARG:HD3 | 2.13                     | 0.49              |
| 40:O:10:LEU:HD23 | 40:O:10:LEU:H    | 1.77                     | 0.49              |
| 40:O:59:LYS:HE3  | 40:O:62:ARG:HH21 | 1.77                     | 0.49              |
| 41:P:74:LYS:HE2  | 41:P:74:LYS:HA   | 1.93                     | 0.49              |
| 47:V:11:VAL:CG1  | 47:V:20:ILE:HD11 | 2.41                     | 0.49              |
| 49:X:14:LEU:HD13 | 49:X:37:SER:CB   | 2.43                     | 0.49              |
| 49:X:44:ILE:HA   | 49:X:61:VAL:CG1  | 2.43                     | 0.49              |
| 51:Z:64:ALA:O    | 51:Z:65:ARG:HB2  | 2.12                     | 0.49              |
| 53:3:77:A:H2'    | 53:3:78:A:C8     | 2.47                     | 0.49              |
| 53:3:422:C:H4'   | 53:3:423:G:N2    | 2.27                     | 0.49              |
| 53:3:1015:G:H2'  | 53:3:1016:A:O4'  | 2.12                     | 0.49              |
| 53:3:1148:U:H6   | 53:3:1148:U:H5'  | 1.77                     | 0.49              |
| 53:3:1227:A:C2'  | 53:3:1228:C:H5'  | 2.40                     | 0.49              |
| 53:3:1444:U:H2'  | 53:3:1445:U:C6   | 2.47                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 54:1:297:G:H2'   | 54:1:298:G:O4'    | 2.12                     | 0.49              |
| 54:1:581:C:H2'   | 54:1:582:A:H8     | 1.77                     | 0.49              |
| 54:1:622:G:O2'   | 54:1:623:C:H5'    | 2.12                     | 0.49              |
| 54:1:671:C:H2'   | 54:1:672:C:C6     | 2.47                     | 0.49              |
| 54:1:704:G:H2'   | 54:1:726:G:N2     | 2.18                     | 0.49              |
| 54:1:1716:U:H2'  | 54:1:1717:A:H8    | 1.78                     | 0.49              |
| 54:1:2869:G:H2'  | 54:1:2870:C:H6    | 1.77                     | 0.49              |
| 59:8:120:GLN:N   | 59:8:121:PRO:HD2  | 2.28                     | 0.49              |
| 1:b:250:GLN:NE2  | 1:b:251:THR:O     | 2.45                     | 0.49              |
| 5:f:46:ASP:CG    | 5:f:48:THR:H      | 2.21                     | 0.49              |
| 37:L:13:PRO:HB3  | 37:L:20:GLU:HG2   | 1.95                     | 0.49              |
| 37:L:79:VAL:HG22 | 53:3:1536:C:O2'   | 2.12                     | 0.49              |
| 37:L:138:GLU:O   | 37:L:142:ARG:HG2  | 2.12                     | 0.49              |
| 38:M:76:ARG:HG2  | 38:M:76:ARG:NH1   | 2.28                     | 0.49              |
| 39:N:27:ILE:HD12 | 39:N:27:ILE:N     | 2.28                     | 0.49              |
| 40:O:71:LEU:N    | 40:O:71:LEU:HD12  | 2.28                     | 0.49              |
| 42:Q:49:ARG:HG2  | 42:Q:49:ARG:NH1   | 2.23                     | 0.49              |
| 47:V:64:ARG:HG2  | 53:3:264:C:O2'    | 2.13                     | 0.49              |
| 53:3:1201:A:H1'  | 53:3:1202:U:OP2   | 2.12                     | 0.49              |
| 53:3:1306:A:H61  | 53:3:1331:G:C2'   | 2.24                     | 0.49              |
| 54:1:549:G:H2'   | 54:1:550:C:H6     | 1.78                     | 0.49              |
| 54:1:880:G:H2'   | 54:1:881:G:C8     | 2.47                     | 0.49              |
| 54:1:2859:G:H2'  | 54:1:2860:A:C8    | 2.47                     | 0.49              |
| 59:8:63:ILE:HG22 | 59:8:63:ILE:O     | 2.13                     | 0.49              |
| 59:8:232:GLU:O   | 59:8:235:GLU:HG3  | 2.12                     | 0.49              |
| 59:8:278:MET:O   | 59:8:282:VAL:HG23 | 2.13                     | 0.49              |
| 2:c:114:LYS:HG3  | 54:1:2680:U:OP1   | 2.13                     | 0.49              |
| 34:I:150:LYS:HE3 | 34:I:155:LYS:HG2  | 1.94                     | 0.49              |
| 36:K:5:GLU:HB2   | 36:K:90:MET:HB2   | 1.94                     | 0.49              |
| 41:P:127:ARG:HB2 | 51:Z:34:ARG:HH22  | 1.78                     | 0.49              |
| 44:S:52:ARG:NH1  | 53:3:1317:C:H42   | 1.98                     | 0.49              |
| 52:a:66:PRO:HD2  | 52:a:188:ASN:OD1  | 2.13                     | 0.49              |
| 53:3:591:U:H2'   | 53:3:592:G:H8     | 1.77                     | 0.49              |
| 54:1:131:A:H2'   | 54:1:132:G:C8     | 2.48                     | 0.49              |
| 54:1:528:A:C2    | 54:1:2042:A:H2'   | 2.48                     | 0.49              |
| 54:1:581:C:H2'   | 54:1:582:A:C8     | 2.47                     | 0.49              |
| 54:1:1810:A:H2'  | 54:1:1811:G:H5'   | 1.94                     | 0.49              |
| 54:1:2554:U:H2'  | 54:1:2555:U:C6    | 2.47                     | 0.49              |
| 54:1:2567:G:H2'  | 54:1:2568:U:C6    | 2.47                     | 0.49              |
| 59:8:136:PRO:HG2 | 59:8:287:PRO:HG3  | 1.93                     | 0.49              |
| 2:c:134:HIS:HE1  | 54:1:1675:C:C4    | 2.31                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:f:122:ALA:HB1   | 5:f:130:ILE:HD11  | 1.95                     | 0.49              |
| 8:i:55:PRO:HD3    | 8:i:74:PRO:CD     | 2.41                     | 0.49              |
| 8:i:57:VAL:O      | 8:i:57:VAL:HG13   | 2.13                     | 0.49              |
| 11:l:116:VAL:HG22 | 11:l:117:THR:N    | 2.28                     | 0.49              |
| 13:n:103:ARG:HE   | 13:n:110:MET:CE   | 2.26                     | 0.49              |
| 17:r:16:GLU:HB2   | 17:r:101:ILE:HG12 | 1.95                     | 0.49              |
| 30:E:37:THR:HA    | 30:E:40:LYS:HB3   | 1.95                     | 0.49              |
| 32:G:31:PHE:N     | 32:G:39:ILE:O     | 2.37                     | 0.49              |
| 38:M:65:PHE:CD2   | 38:M:66:GLN:HG2   | 2.47                     | 0.49              |
| 41:P:126:ARG:NH2  | 53:3:692:U:H5''   | 2.16                     | 0.49              |
| 44:S:12:ARG:HG2   | 44:S:59:GLN:CG    | 2.43                     | 0.49              |
| 53:3:890:G:H2'    | 53:3:906:A:N6     | 2.28                     | 0.49              |
| 53:3:923:A:H2'    | 53:3:924:C:C6     | 2.48                     | 0.49              |
| 53:3:1200:C:C5'   | 53:3:1201:A:H3'   | 2.40                     | 0.49              |
| 54:1:26:G:O2'     | 54:1:27:G:H5'     | 2.11                     | 0.49              |
| 54:1:616:A:H2'    | 54:1:617:G:O4'    | 2.13                     | 0.49              |
| 54:1:969:G:H2'    | 54:1:970:U:C6     | 2.48                     | 0.49              |
| 54:1:1077:A:H2'   | 54:1:1078:U:H5'   | 1.94                     | 0.49              |
| 54:1:2224:G:H4'   | 54:1:2226:C:C2    | 2.47                     | 0.49              |
| 54:1:2238:G:H2'   | 54:1:2238:G:N3    | 2.28                     | 0.49              |
| 54:1:2514:U:H2'   | 54:1:2515:C:C6    | 2.48                     | 0.49              |
| 54:1:2795:C:H2'   | 54:1:2796:U:O4'   | 2.13                     | 0.49              |
| 59:8:295:ILE:HG21 | 59:8:309:ARG:NH2  | 2.27                     | 0.49              |
| 59:8:502:GLU:HB3  | 59:8:519:VAL:HG12 | 1.94                     | 0.49              |
| 59:8:505:HIS:O    | 59:8:515:TYR:HA   | 2.13                     | 0.49              |
| 2:c:25:THR:HG21   | 2:c:193:VAL:HG22  | 1.95                     | 0.48              |
| 7:h:11:ILE:O      | 7:h:15:VAL:HG23   | 2.13                     | 0.48              |
| 10:k:105:ARG:O    | 10:k:107:LEU:N    | 2.43                     | 0.48              |
| 13:n:35:LYS:HZ3   | 13:n:110:MET:HE3  | 1.78                     | 0.48              |
| 21:v:57:TYR:HA    | 21:v:74:ALA:HB3   | 1.94                     | 0.48              |
| 24:y:57:LEU:HD23  | 24:y:57:LEU:C     | 2.38                     | 0.48              |
| 33:H:185:THR:HG23 | 33:H:197:VAL:O    | 2.13                     | 0.48              |
| 37:L:138:GLU:O    | 37:L:142:ARG:N    | 2.46                     | 0.48              |
| 41:P:28:ASN:OD1   | 41:P:56:LYS:HD3   | 2.13                     | 0.48              |
| 44:S:20:PHE:HZ    | 44:S:27:LYS:HE2   | 1.77                     | 0.48              |
| 49:X:5:LYS:HA     | 53:3:1313:U:H5''  | 1.93                     | 0.48              |
| 49:X:40:PHE:HB2   | 49:X:42:ASN:OD1   | 2.13                     | 0.48              |
| 53:3:259:G:H2'    | 53:3:260:G:O4'    | 2.13                     | 0.48              |
| 53:3:371:A:H2'    | 53:3:372:C:O4'    | 2.13                     | 0.48              |
| 53:3:544:G:H2'    | 53:3:545:C:C6     | 2.48                     | 0.48              |
| 53:3:1280:A:H5'   | 53:3:1280:A:H8    | 1.77                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:1523:G:H2'   | 53:3:1524:C:C6    | 2.47                     | 0.48              |
| 54:1:588:U:H2'    | 54:1:589:U:C6     | 2.48                     | 0.48              |
| 54:1:727:A:H2'    | 54:1:728:G:C8     | 2.48                     | 0.48              |
| 54:1:894:U:H2'    | 54:1:895:U:C6     | 2.48                     | 0.48              |
| 54:1:1196:C:H2'   | 54:1:1197:G:C8    | 2.48                     | 0.48              |
| 54:1:1683:U:H2'   | 54:1:1684:G:H8    | 1.78                     | 0.48              |
| 54:1:2619:C:O2'   | 54:1:2620:C:H5'   | 2.13                     | 0.48              |
| 59:8:31:LEU:HA    | 59:8:34:THR:OG1   | 2.13                     | 0.48              |
| 59:8:130:ALA:O    | 59:8:134:LYS:N    | 2.45                     | 0.48              |
| 59:8:152:LEU:HA   | 59:8:155:VAL:HG22 | 1.95                     | 0.48              |
| 59:8:152:LEU:HD23 | 59:8:152:LEU:N    | 2.27                     | 0.48              |
| 1:b:52:HIS:ND1    | 1:b:52:HIS:N      | 2.61                     | 0.48              |
| 8:i:12:VAL:HG22   | 54:1:1061:U:O2    | 2.13                     | 0.48              |
| 10:k:109:SER:O    | 10:k:110:GLU:HB3  | 2.13                     | 0.48              |
| 22:w:68:LYS:HB2   | 22:w:75:PHE:CD2   | 2.48                     | 0.48              |
| 32:G:136:ARG:HH11 | 32:G:136:ARG:CB   | 2.20                     | 0.48              |
| 32:G:186:VAL:HG22 | 32:G:199:ILE:O    | 2.13                     | 0.48              |
| 33:H:177:LEU:HB2  | 53:3:1112:C:N3    | 2.28                     | 0.48              |
| 34:I:12:ARG:CB    | 34:I:12:ARG:HH11  | 2.26                     | 0.48              |
| 35:J:81:GLN:H     | 35:J:146:MET:HE1  | 1.78                     | 0.48              |
| 35:J:159:SER:HB2  | 35:J:162:GLU:HB2  | 1.95                     | 0.48              |
| 39:N:38:PHE:HZ    | 39:N:47:VAL:HG11  | 1.79                     | 0.48              |
| 41:P:93:GLU:HG2   | 41:P:97:ARG:NH2   | 2.27                     | 0.48              |
| 41:P:116:PRO:O    | 41:P:118:ASN:N    | 2.44                     | 0.48              |
| 42:Q:109:ARG:CB   | 42:Q:118:VAL:HG21 | 2.35                     | 0.48              |
| 42:Q:110:LYS:HB2  | 53:3:538:G:H5''   | 1.94                     | 0.48              |
| 47:V:45:VAL:HG12  | 47:V:46:HIS:N     | 2.29                     | 0.48              |
| 47:V:64:ARG:HB3   | 47:V:64:ARG:NH1   | 2.27                     | 0.48              |
| 52:a:60:ARG:HH21  | 52:a:164:ARG:NH1  | 2.11                     | 0.48              |
| 53:3:426:U:H2'    | 53:3:427:U:C6     | 2.48                     | 0.48              |
| 53:3:571:U:H3'    | 53:3:572:A:H5''   | 1.95                     | 0.48              |
| 54:1:64:A:H2'     | 54:1:65:U:C6      | 2.48                     | 0.48              |
| 54:1:69:C:O2'     | 54:1:70:G:H5'     | 2.13                     | 0.48              |
| 54:1:75:G:H2'     | 54:1:75:G:N3      | 2.26                     | 0.48              |
| 54:1:149:A:H2'    | 54:1:150:U:C6     | 2.48                     | 0.48              |
| 54:1:445:C:C2'    | 54:1:446:G:H5'    | 2.43                     | 0.48              |
| 54:1:521:U:H2'    | 54:1:522:A:H8     | 1.78                     | 0.48              |
| 54:1:1443:U:H2'   | 54:1:1444:G:H8    | 1.77                     | 0.48              |
| 54:1:1710:G:H2'   | 54:1:1711:A:C8    | 2.48                     | 0.48              |
| 54:1:2020:A:O2'   | 54:1:2021:C:H5'   | 2.14                     | 0.48              |
| 54:1:2788:C:H2'   | 54:1:2789:C:H6    | 1.77                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:2884:U:O2    | 54:1:2884:U:H3'   | 2.13                     | 0.48              |
| 3:d:149:ILE:CG2   | 3:d:188:MET:HA    | 2.44                     | 0.48              |
| 8:i:23:VAL:CG1    | 8:i:26:ALA:HB3    | 2.43                     | 0.48              |
| 9:j:16:TYR:HB2    | 9:j:54:ILE:HD12   | 1.95                     | 0.48              |
| 11:l:19:LEU:HD11  | 11:l:31:GLY:O     | 2.12                     | 0.48              |
| 12:m:100:LYS:O    | 12:m:102:LEU:HD22 | 2.13                     | 0.48              |
| 15:p:24:THR:HB    | 15:p:86:LYS:HB2   | 1.95                     | 0.48              |
| 22:w:22:PHE:CD2   | 54:1:922:C:H1'    | 2.49                     | 0.48              |
| 36:K:54:LEU:HD23  | 36:K:54:LEU:N     | 2.28                     | 0.48              |
| 39:N:11:ARG:NH1   | 39:N:12:LYS:HB2   | 2.28                     | 0.48              |
| 47:V:20:ILE:O     | 47:V:45:VAL:N     | 2.39                     | 0.48              |
| 52:a:40:GLU:H     | 52:a:178:VAL:CG2  | 2.26                     | 0.48              |
| 53:3:86:G:H4'     | 53:3:87:C:C5      | 2.48                     | 0.48              |
| 53:3:651:C:H2'    | 53:3:652:U:C6     | 2.49                     | 0.48              |
| 53:3:710:G:O2'    | 53:3:711:G:H5'    | 2.13                     | 0.48              |
| 53:3:1158:C:C4    | 53:3:1160:G:H1'   | 2.48                     | 0.48              |
| 54:1:704:G:C2'    | 54:1:726:G:H22    | 2.16                     | 0.48              |
| 54:1:786:C:O2'    | 54:1:787:C:H5'    | 2.13                     | 0.48              |
| 54:1:1075:C:C2'   | 54:1:1076:C:H5''  | 2.43                     | 0.48              |
| 54:1:1554:U:O2'   | 54:1:1555:G:H5''  | 2.13                     | 0.48              |
| 54:1:1572:A:H2'   | 54:1:1573:G:H8    | 1.79                     | 0.48              |
| 55:2:2:G:H2'      | 55:2:3:C:H6       | 1.77                     | 0.48              |
| 55:2:59:A:H2'     | 55:2:60:C:O4'     | 2.13                     | 0.48              |
| 59:8:104:ARG:NH2  | 59:8:105:VAL:HG12 | 2.28                     | 0.48              |
| 59:8:137:ARG:HG3  | 59:8:262:ILE:CG2  | 2.44                     | 0.48              |
| 1:b:53:ILE:O      | 1:b:216:ARG:HD3   | 2.13                     | 0.48              |
| 2:c:1:MET:HG3     | 2:c:205:PRO:HG2   | 1.94                     | 0.48              |
| 11:l:122:VAL:HG22 | 11:l:123:ARG:N    | 2.28                     | 0.48              |
| 13:n:65:LEU:O     | 13:n:68:ALA:HB3   | 2.13                     | 0.48              |
| 14:o:31:THR:HG23  | 14:o:32:PRO:CD    | 2.42                     | 0.48              |
| 21:v:7:GLU:O      | 21:v:40:ILE:HG23  | 2.14                     | 0.48              |
| 34:I:75:TYR:CZ    | 34:I:203:TYR:HB3  | 2.49                     | 0.48              |
| 36:K:23:GLU:HA    | 36:K:26:THR:HG22  | 1.94                     | 0.48              |
| 36:K:24:ARG:HB2   | 36:K:24:ARG:HH11  | 1.78                     | 0.48              |
| 49:X:52:ASN:C     | 49:X:54:ARG:H     | 2.21                     | 0.48              |
| 53:3:110:C:H2'    | 53:3:111:G:O4'    | 2.14                     | 0.48              |
| 53:3:291:U:O2'    | 53:3:292:G:H5'    | 2.13                     | 0.48              |
| 53:3:1334:G:H2'   | 53:3:1335:U:C5'   | 2.40                     | 0.48              |
| 53:3:1500:A:H5''  | 53:3:1508:A:H5''  | 1.94                     | 0.48              |
| 54:1:74:A:H4'     | 54:1:75:G:O5'     | 2.14                     | 0.48              |
| 54:1:705:A:H2'    | 54:1:706:A:C8     | 2.46                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:1400:U:H2'   | 54:1:1401:G:H8    | 1.78                     | 0.48              |
| 54:1:2129:C:H2'   | 54:1:2159:G:N2    | 2.27                     | 0.48              |
| 54:1:2679:A:H2'   | 54:1:2680:U:C6    | 2.47                     | 0.48              |
| 59:8:137:ARG:HG3  | 59:8:262:ILE:HG22 | 1.95                     | 0.48              |
| 59:8:175:ALA:H    | 59:8:178:HIS:HB2  | 1.78                     | 0.48              |
| 1:b:1:ALA:N       | 1:b:19:VAL:O      | 2.39                     | 0.48              |
| 3:d:32:VAL:HG11   | 11:l:6:LEU:CD1    | 2.43                     | 0.48              |
| 6:g:40:THR:O      | 6:g:42:LYS:N      | 2.36                     | 0.48              |
| 9:j:120:ARG:HG3   | 9:j:120:ARG:NH2   | 2.28                     | 0.48              |
| 13:n:30:ARG:HH12  | 13:n:75:ILE:HD11  | 1.77                     | 0.48              |
| 22:w:67:VAL:HG23  | 22:w:67:VAL:O     | 2.13                     | 0.48              |
| 23:x:35:HIS:CG    | 23:x:36:ARG:N     | 2.82                     | 0.48              |
| 25:z:14:GLY:O     | 25:z:15:ARG:HD3   | 2.14                     | 0.48              |
| 32:G:59:ILE:CD1   | 32:G:159:ALA:HB2  | 2.43                     | 0.48              |
| 34:I:124:VAL:HG22 | 34:I:125:ASN:HD22 | 1.78                     | 0.48              |
| 35:J:14:LEU:HD23  | 35:J:15:ILE:N     | 2.28                     | 0.48              |
| 38:M:64:TYR:CE1   | 38:M:69:ALA:HB2   | 2.48                     | 0.48              |
| 51:Z:44:ARG:CZ    | 51:Z:45:LYS:HA    | 2.43                     | 0.48              |
| 52:a:60:ARG:NE    | 52:a:164:ARG:HH11 | 2.04                     | 0.48              |
| 52:a:212:VAL:HB   | 52:a:224:VAL:CG2  | 2.44                     | 0.48              |
| 53:3:147:G:H2'    | 53:3:148:G:H8     | 1.74                     | 0.48              |
| 53:3:222:C:H2'    | 53:3:223:A:H8     | 1.78                     | 0.48              |
| 53:3:951:G:H2'    | 53:3:952:U:H6     | 1.79                     | 0.48              |
| 54:1:290:U:H2'    | 54:1:291:G:H8     | 1.79                     | 0.48              |
| 54:1:323:C:H2'    | 54:1:1205:A:N1    | 2.29                     | 0.48              |
| 54:1:1409:U:H2'   | 54:1:1410:G:C8    | 2.49                     | 0.48              |
| 54:1:1707:G:H2'   | 54:1:1708:C:C6    | 2.48                     | 0.48              |
| 54:1:1726:C:H2'   | 54:1:1727:C:C6    | 2.48                     | 0.48              |
| 59:8:20:ASP:N     | 62:8:801:GCP:H3B1 | 2.17                     | 0.48              |
| 59:8:168:PRO:C    | 59:8:170:GLN:H    | 2.20                     | 0.48              |
| 2:c:52:THR:O      | 2:c:77:ARG:HG2    | 2.14                     | 0.48              |
| 2:c:97:SER:O      | 2:c:100:LEU:HD13  | 2.13                     | 0.48              |
| 10:k:43:ILE:HD12  | 10:k:43:ILE:N     | 2.28                     | 0.48              |
| 30:E:24:LYS:HG2   | 30:E:25:HIS:N     | 2.29                     | 0.48              |
| 35:J:59:ILE:HG13  | 35:J:60:GLN:N     | 2.28                     | 0.48              |
| 35:J:86:GLY:N     | 35:J:93:VAL:O     | 2.40                     | 0.48              |
| 40:O:61:ALA:HB1   | 53:3:1061:G:OP1   | 2.13                     | 0.48              |
| 42:Q:34:THR:HG23  | 42:Q:53:ARG:HE    | 1.78                     | 0.48              |
| 47:V:10:ARG:HA    | 47:V:56:ASP:O     | 2.12                     | 0.48              |
| 53:3:346:G:C2'    | 53:3:347:G:H5'    | 2.43                     | 0.48              |
| 53:3:449:G:H2'    | 53:3:450:G:C8     | 2.48                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:3:764:C:H2'   | 53:3:765:G:O4'    | 2.13                     | 0.48              |
| 54:1:1137:G:O2'  | 54:1:1138:G:H5'   | 2.13                     | 0.48              |
| 54:1:1308:A:H2'  | 54:1:1309:G:C5'   | 2.42                     | 0.48              |
| 59:8:23:LYS:HE3  | 59:8:90:PRO:HG2   | 1.94                     | 0.48              |
| 59:8:92:HIS:H    | 59:8:95:PHE:HD2   | 1.62                     | 0.48              |
| 59:8:253:ARG:O   | 59:8:257:LEU:HD13 | 2.13                     | 0.48              |
| 1:b:61:TYR:CE1   | 54:1:1816:C:H3'   | 2.48                     | 0.48              |
| 1:b:152:GLN:HB3  | 54:1:1818:U:C4    | 2.49                     | 0.48              |
| 6:g:5:LEU:CD1    | 6:g:13:GLY:HA2    | 2.43                     | 0.48              |
| 9:j:110:PRO:O    | 9:j:115:GLY:HA3   | 2.13                     | 0.48              |
| 11:l:42:SER:HB2  | 54:1:672:C:H5     | 1.78                     | 0.48              |
| 14:o:67:ASN:HA   | 55:2:50:A:OP2     | 2.14                     | 0.48              |
| 20:u:11:ILE:HD11 | 20:u:19:GLY:C     | 2.39                     | 0.48              |
| 21:v:30:ILE:HA   | 21:v:91:PHE:HB2   | 1.96                     | 0.48              |
| 28:C:27:ARG:HH11 | 28:C:27:ARG:HB2   | 1.77                     | 0.48              |
| 34:I:183:ARG:HD3 | 34:I:183:ARG:N    | 2.28                     | 0.48              |
| 39:N:99:LYS:N    | 39:N:99:LYS:HD2   | 2.29                     | 0.48              |
| 40:O:6:ILE:HD12  | 40:O:102:LEU:HA   | 1.95                     | 0.48              |
| 42:Q:38:THR:CG2  | 42:Q:48:LEU:HG    | 2.42                     | 0.48              |
| 43:R:69:ARG:CB   | 43:R:69:ARG:HH11  | 2.26                     | 0.48              |
| 45:T:20:ASP:OD1  | 53:3:751:U:H5'    | 2.13                     | 0.48              |
| 50:Y:2:ASN:ND2   | 50:Y:3:ILE:HG13   | 2.28                     | 0.48              |
| 50:Y:66:ILE:HG23 | 50:Y:70:LYS:HB3   | 1.94                     | 0.48              |
| 53:3:236:A:H2'   | 53:3:237:G:H8     | 1.79                     | 0.48              |
| 53:3:853:C:H2'   | 53:3:854:U:H6     | 1.78                     | 0.48              |
| 53:3:1082:A:H2'  | 53:3:1083:U:O4'   | 2.13                     | 0.48              |
| 53:3:1122:U:C2'  | 53:3:1123:U:C5    | 2.92                     | 0.48              |
| 54:1:150:U:H2'   | 54:1:151:C:C6     | 2.48                     | 0.48              |
| 54:1:800:A:N1    | 54:1:802:A:C8     | 2.81                     | 0.48              |
| 54:1:937:C:H2'   | 54:1:938:G:H8     | 1.78                     | 0.48              |
| 54:1:1306:C:N4   | 54:1:1606:C:H2'   | 2.29                     | 0.48              |
| 54:1:2400:G:O2'  | 54:1:2401:U:H5'   | 2.14                     | 0.48              |
| 59:8:128:ARG:O   | 59:8:132:LYS:N    | 2.46                     | 0.48              |
| 59:8:473:MET:HA  | 59:8:477:PHE:HB2  | 1.96                     | 0.48              |
| 1:b:222:THR:HG23 | 54:1:1826:G:OP1   | 2.14                     | 0.48              |
| 3:d:98:LYS:HG3   | 54:1:607:U:P      | 2.53                     | 0.48              |
| 11:l:93:ASN:O    | 11:l:94:THR:CB    | 2.62                     | 0.48              |
| 16:q:80:ASN:HD22 | 54:1:1151:A:H4'   | 1.77                     | 0.48              |
| 33:H:4:VAL:HG21  | 44:S:97:LYS:NZ    | 2.28                     | 0.48              |
| 37:L:90:VAL:HG22 | 37:L:91:ARG:N     | 2.28                     | 0.48              |
| 43:R:95:PRO:CB   | 53:3:1307:U:O3'   | 2.61                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 43:R:97:ARG:HA    | 53:3:1308:U:C6   | 2.49                     | 0.48              |
| 50:Y:82:ILE:HG13  | 50:Y:83:ASN:N    | 2.27                     | 0.48              |
| 53:3:15:G:N2      | 53:3:1080:A:C1'  | 2.74                     | 0.48              |
| 53:3:538:G:H2'    | 53:3:539:A:H8    | 1.78                     | 0.48              |
| 53:3:555:U:H2'    | 53:3:556:C:H6    | 1.76                     | 0.48              |
| 53:3:563:A:H61    | 53:3:884:U:H3    | 1.62                     | 0.48              |
| 53:3:979:C:C2     | 53:3:1318:A:N1   | 2.82                     | 0.48              |
| 53:3:1165:U:O2    | 53:3:1165:U:H2'  | 2.14                     | 0.48              |
| 53:3:1252:A:H61   | 53:3:1285:A:H61  | 1.62                     | 0.48              |
| 53:3:1360:A:O2'   | 53:3:1361:G:H5'  | 2.14                     | 0.48              |
| 54:1:792:A:H2'    | 54:1:2440:C:O2   | 2.14                     | 0.48              |
| 54:1:1002:G:H2'   | 54:1:1003:G:O4'  | 2.12                     | 0.48              |
| 54:1:2743:U:C2'   | 54:1:2744:G:H5'' | 2.41                     | 0.48              |
| 59:8:498:VAL:HG22 | 59:8:499:THR:H   | 1.79                     | 0.48              |
| 59:8:605:PHE:CE1  | 59:8:610:PRO:HG2 | 2.49                     | 0.48              |
| 3:d:52:VAL:HG21   | 3:d:82:GLY:N     | 2.24                     | 0.48              |
| 3:d:63:LYS:HE2    | 54:1:2444:G:P    | 2.53                     | 0.48              |
| 6:g:31:VAL:N      | 6:g:32:PRO:HD2   | 2.29                     | 0.48              |
| 12:m:35:ALA:HB2   | 12:m:102:LEU:CD2 | 2.44                     | 0.48              |
| 12:m:45:GLN:NE2   | 12:m:125:PRO:HD3 | 2.28                     | 0.48              |
| 14:o:24:THR:HG23  | 14:o:40:ILE:O    | 2.14                     | 0.48              |
| 20:u:13:LEU:HB2   | 20:u:68:ASN:O    | 2.13                     | 0.48              |
| 20:u:46:LYS:NZ    | 20:u:48:VAL:HA   | 2.29                     | 0.48              |
| 25:z:5:LYS:HB2    | 25:z:57:GLU:CG   | 2.43                     | 0.48              |
| 34:I:142:VAL:O    | 34:I:179:GLY:N   | 2.47                     | 0.48              |
| 52:a:23:ILE:HG22  | 52:a:186:LYS:HG2 | 1.96                     | 0.48              |
| 52:a:218:MET:HE2  | 54:1:2174:C:H1'  | 1.96                     | 0.48              |
| 53:3:1436:U:H2'   | 53:3:1437:A:C8   | 2.48                     | 0.48              |
| 54:1:15:G:O2'     | 54:1:16:C:H5'    | 2.14                     | 0.48              |
| 54:1:460:A:H2'    | 54:1:461:C:O4'   | 2.14                     | 0.48              |
| 54:1:1075:C:C3'   | 54:1:1076:C:C5'  | 2.89                     | 0.48              |
| 54:1:2492:U:H2'   | 54:1:2493:U:C6   | 2.48                     | 0.48              |
| 54:1:2661:G:O2'   | 54:1:2662:A:H5'  | 2.13                     | 0.48              |
| 55:2:106:G:H2'    | 55:2:107:G:O4'   | 2.14                     | 0.48              |
| 59:8:72:TRP:CD1   | 59:8:279:LEU:HG  | 2.48                     | 0.48              |
| 59:8:159:LYS:HZ3  | 59:8:166:PRO:HD2 | 1.79                     | 0.48              |
| 1:b:77:VAL:HG21   | 1:b:109:LEU:CD2  | 2.44                     | 0.48              |
| 1:b:229:HIS:CG    | 1:b:230:PRO:HD2  | 2.49                     | 0.48              |
| 5:f:9:VAL:HA      | 5:f:48:THR:CB    | 2.43                     | 0.48              |
| 15:p:29:VAL:HG12  | 15:p:30:TRP:O    | 2.14                     | 0.48              |
| 19:t:14:PRO:HA    | 19:t:32:LEU:HB3  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:G:49:PHE:CD1   | 32:G:49:PHE:C     | 2.92                     | 0.48              |
| 35:J:67:ARG:HB2   | 35:J:67:ARG:CZ    | 2.44                     | 0.48              |
| 35:J:105:ILE:HD11 | 35:J:123:LEU:HB3  | 1.95                     | 0.48              |
| 35:J:110:MET:O    | 35:J:114:LEU:HD23 | 2.13                     | 0.48              |
| 36:K:38:ARG:NE    | 36:K:40:GLU:HG3   | 2.29                     | 0.48              |
| 37:L:14:ASP:HB3   | 37:L:15:PRO:HD2   | 1.95                     | 0.48              |
| 38:M:94:VAL:CG2   | 38:M:101:ALA:HB2  | 2.44                     | 0.48              |
| 39:N:49:GLN:N     | 39:N:50:PRO:HD2   | 2.28                     | 0.48              |
| 42:Q:86:VAL:CG2   | 42:Q:89:LEU:H     | 2.26                     | 0.48              |
| 44:S:60:ARG:HG2   | 44:S:61:ASN:N     | 2.29                     | 0.48              |
| 47:V:27:PHE:CE2   | 47:V:36:PHE:HB3   | 2.49                     | 0.48              |
| 53:3:585:G:H2'    | 53:3:586:C:H6     | 1.78                     | 0.48              |
| 53:3:603:U:H2'    | 53:3:604:G:C8     | 2.48                     | 0.48              |
| 53:3:1336:C:H4'   | 53:3:1337:G:C4    | 2.49                     | 0.48              |
| 54:1:563:A:H2'    | 54:1:564:C:H6     | 1.79                     | 0.48              |
| 54:1:608:A:H2'    | 54:1:609:A:H8     | 1.79                     | 0.48              |
| 54:1:669:G:H2'    | 54:1:669:G:N3     | 2.29                     | 0.48              |
| 54:1:2081:U:H2'   | 54:1:2082:A:H8    | 1.78                     | 0.48              |
| 54:1:2089:C:O2'   | 54:1:2090:A:H5'   | 2.14                     | 0.48              |
| 54:1:2155:U:C2'   | 54:1:2156:G:H5'   | 2.42                     | 0.48              |
| 54:1:2888:C:H2'   | 54:1:2889:C:C6    | 2.49                     | 0.48              |
| 56:5:2:G:HO2'     | 56:5:3:G:H2'      | 1.77                     | 0.48              |
| 59:8:420:VAL:HG12 | 59:8:483:VAL:HA   | 1.96                     | 0.48              |
| 7:h:41:LEU:HB3    | 54:1:1083:U:OP1   | 2.14                     | 0.47              |
| 8:i:55:PRO:HD3    | 8:i:73:PRO:HA     | 1.96                     | 0.47              |
| 9:j:135:GLN:NE2   | 54:1:7:G:H1'      | 2.29                     | 0.47              |
| 15:p:105:LYS:CD   | 15:p:108:ARG:HD3  | 2.44                     | 0.47              |
| 17:r:74:ILE:HB    | 17:r:87:GLN:O     | 2.14                     | 0.47              |
| 19:t:12:ARG:HH11  | 19:t:12:ARG:HG3   | 1.79                     | 0.47              |
| 32:G:57:ASN:O     | 32:G:61:SER:N     | 2.42                     | 0.47              |
| 33:H:115:VAL:HG12 | 33:H:119:ILE:HD11 | 1.97                     | 0.47              |
| 34:I:72:ARG:O     | 34:I:72:ARG:HD2   | 2.14                     | 0.47              |
| 34:I:131:ILE:HG12 | 53:3:620:C:C2     | 2.49                     | 0.47              |
| 37:L:102:TRP:CZ2  | 37:L:140:VAL:HG21 | 2.49                     | 0.47              |
| 38:M:82:LEU:C     | 38:M:82:LEU:HD23  | 2.39                     | 0.47              |
| 39:N:88:GLU:HG2   | 39:N:89:TYR:N     | 2.28                     | 0.47              |
| 41:P:22:ILE:HG21  | 41:P:95:THR:HG21  | 1.96                     | 0.47              |
| 45:T:88:ARG:HH12  | 54:1:715:A:H5''   | 1.79                     | 0.47              |
| 48:W:35:SER:HB3   | 51:Z:18:PHE:CE2   | 2.48                     | 0.47              |
| 49:X:52:ASN:HD22  | 49:X:57:VAL:CG1   | 2.27                     | 0.47              |
| 50:Y:2:ASN:CG     | 50:Y:3:ILE:N      | 2.69                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:1405:G:O2'   | 53:3:1406:U:H5'   | 2.14                     | 0.47              |
| 54:1:689:A:H2'    | 54:1:690:G:C8     | 2.48                     | 0.47              |
| 54:1:809:G:C6     | 54:1:810:U:N3     | 2.82                     | 0.47              |
| 54:1:1442:U:H2'   | 54:1:1443:U:C6    | 2.48                     | 0.47              |
| 54:1:1824:G:H2'   | 54:1:1825:U:H6    | 1.79                     | 0.47              |
| 54:1:1890:A:H2'   | 54:1:1891:G:O4'   | 2.14                     | 0.47              |
| 54:1:2393:U:H2'   | 54:1:2394:C:C6    | 2.49                     | 0.47              |
| 54:1:2626:C:H2'   | 54:1:2627:G:H8    | 1.79                     | 0.47              |
| 59:8:282:VAL:CG1  | 59:8:286:LEU:HD22 | 2.40                     | 0.47              |
| 59:8:371:ARG:HD2  | 59:8:371:ARG:N    | 2.29                     | 0.47              |
| 59:8:645:GLN:NE2  | 59:8:645:GLN:O    | 2.47                     | 0.47              |
| 1:b:120:ASP:HB2   | 6:g:91:PHE:HE1    | 1.79                     | 0.47              |
| 4:e:147:ARG:HD3   | 4:e:148:VAL:H     | 1.78                     | 0.47              |
| 5:f:88:LEU:CD2    | 5:f:93:TYR:HB3    | 2.44                     | 0.47              |
| 10:k:43:ILE:HD11  | 10:k:58:LEU:HD21  | 1.95                     | 0.47              |
| 12:m:4:PRO:HG2    | 12:m:70:ASP:HA    | 1.96                     | 0.47              |
| 22:w:51:ARG:HH11  | 22:w:51:ARG:HG3   | 1.77                     | 0.47              |
| 23:x:63:ILE:HG23  | 23:x:64:ASP:H     | 1.79                     | 0.47              |
| 28:C:17:GLY:O     | 28:C:19:PHE:HD1   | 1.97                     | 0.47              |
| 30:E:39:ARG:O     | 30:E:43:LEU:HD13  | 2.14                     | 0.47              |
| 32:G:153:MET:HE2  | 32:G:155:GLY:O    | 2.14                     | 0.47              |
| 33:H:159:ALA:C    | 33:H:161:ILE:H    | 2.22                     | 0.47              |
| 36:K:62:MET:SD    | 36:K:62:MET:N     | 2.88                     | 0.47              |
| 38:M:124:ILE:HD11 | 38:M:127:TYR:HE1  | 1.78                     | 0.47              |
| 42:Q:2:THR:O      | 42:Q:5:GLN:N      | 2.47                     | 0.47              |
| 42:Q:23:LEU:HD12  | 42:Q:29:LYS:NZ    | 2.26                     | 0.47              |
| 43:R:19:THR:HA    | 43:R:24:VAL:HG23  | 1.96                     | 0.47              |
| 49:X:2:ARG:N      | 53:3:1313:U:O4    | 2.47                     | 0.47              |
| 53:3:1122:U:H2'   | 53:3:1123:U:H5    | 1.71                     | 0.47              |
| 53:3:1360:A:H2'   | 53:3:1361:G:O4'   | 2.15                     | 0.47              |
| 53:3:1493:A:O2'   | 53:3:1494:G:OP1   | 2.27                     | 0.47              |
| 54:1:290:U:H2'    | 54:1:291:G:C8     | 2.49                     | 0.47              |
| 54:1:483:A:H2'    | 54:1:484:C:O4'    | 2.14                     | 0.47              |
| 54:1:765:C:H2'    | 54:1:766:U:C6     | 2.49                     | 0.47              |
| 54:1:841:G:H2'    | 54:1:842:U:C6     | 2.50                     | 0.47              |
| 54:1:1298:C:H2'   | 54:1:1299:G:O4'   | 2.14                     | 0.47              |
| 54:1:2126:A:H2'   | 54:1:2162:G:N2    | 2.28                     | 0.47              |
| 59:8:158:ILE:O    | 59:8:163:GLY:N    | 2.47                     | 0.47              |
| 59:8:174:GLY:HA3  | 59:8:178:HIS:O    | 2.14                     | 0.47              |
| 59:8:189:LYS:HE3  | 59:8:204:TYR:CD1  | 2.48                     | 0.47              |
| 59:8:220:GLN:HA   | 59:8:223:ILE:HG12 | 1.96                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 20:u:46:LYS:HD2   | 20:u:47:PRO:C    | 2.39                     | 0.47              |
| 26:A:62:LYS:HD3   | 49:X:16:LYS:CB   | 2.44                     | 0.47              |
| 29:D:30:VAL:HA    | 29:D:33:ARG:NH1  | 2.30                     | 0.47              |
| 35:J:104:ILE:HG23 | 35:J:104:ILE:O   | 2.14                     | 0.47              |
| 36:K:6:ILE:HD11   | 36:K:78:PHE:CZ   | 2.50                     | 0.47              |
| 42:Q:86:VAL:HG23  | 42:Q:89:LEU:H    | 1.80                     | 0.47              |
| 43:R:97:ARG:HG3   | 53:3:1308:U:H1'  | 1.96                     | 0.47              |
| 52:a:50:ILE:HG23  | 52:a:208:TYR:HA  | 1.96                     | 0.47              |
| 53:3:626:G:H2'    | 53:3:627:G:C8    | 2.49                     | 0.47              |
| 53:3:943:U:H6     | 53:3:943:U:O5'   | 1.96                     | 0.47              |
| 53:3:945:G:H1'    | 53:3:1337:G:H1'  | 1.95                     | 0.47              |
| 53:3:945:G:H2'    | 53:3:945:G:N3    | 2.28                     | 0.47              |
| 54:1:851:C:H2'    | 54:1:852:U:H6    | 1.79                     | 0.47              |
| 54:1:1476:U:H3    | 54:1:1515:A:H62  | 1.60                     | 0.47              |
| 54:1:1921:G:O2'   | 54:1:1922:G:H5'  | 2.15                     | 0.47              |
| 54:1:2246:G:H2'   | 54:1:2247:A:C8   | 2.49                     | 0.47              |
| 54:1:2555:U:H2'   | 54:1:2556:C:H5'  | 1.95                     | 0.47              |
| 55:2:63:C:H2'     | 55:2:64:G:C8     | 2.49                     | 0.47              |
| 2:c:181:ASP:HB3   | 2:c:186:LEU:HB2  | 1.96                     | 0.47              |
| 4:e:28:PRO:HB3    | 4:e:159:ALA:HA   | 1.97                     | 0.47              |
| 4:e:92:GLY:O      | 4:e:95:MET:HB3   | 2.14                     | 0.47              |
| 11:l:63:LYS:HA    | 30:E:12:ARG:HG2  | 1.95                     | 0.47              |
| 11:l:111:ILE:HG22 | 11:l:112:LEU:N   | 2.29                     | 0.47              |
| 13:n:12:ARG:HD3   | 13:n:16:HIS:CD2  | 2.48                     | 0.47              |
| 22:w:14:ALA:HB1   | 54:1:2271:G:OP1  | 2.15                     | 0.47              |
| 22:w:17:LEU:H     | 22:w:17:LEU:CD1  | 2.27                     | 0.47              |
| 22:w:17:LEU:HD11  | 22:w:37:ARG:NH2  | 2.29                     | 0.47              |
| 32:G:59:ILE:HD12  | 32:G:159:ALA:HB2 | 1.95                     | 0.47              |
| 32:G:80:LYS:HG3   | 32:G:90:PHE:CZ   | 2.49                     | 0.47              |
| 32:G:91:VAL:HG21  | 32:G:99:MET:HE1  | 1.95                     | 0.47              |
| 32:G:119:GLN:HB3  | 32:G:124:THR:H   | 1.79                     | 0.47              |
| 32:G:160:LEU:HD22 | 32:G:175:ALA:HB3 | 1.97                     | 0.47              |
| 33:H:153:SER:O    | 33:H:196:GLY:N   | 2.47                     | 0.47              |
| 34:I:15:GLY:CA    | 34:I:34:GLU:HG3  | 2.45                     | 0.47              |
| 37:L:91:ARG:HG2   | 37:L:91:ARG:NH1  | 2.27                     | 0.47              |
| 37:L:115:MET:HE2  | 53:3:1240:U:O4'  | 2.14                     | 0.47              |
| 38:M:76:ARG:HD2   | 38:M:125:ILE:O   | 2.15                     | 0.47              |
| 40:O:46:LYS:HG2   | 40:O:68:ARG:CB   | 2.45                     | 0.47              |
| 45:T:47:LYS:O     | 45:T:49:HIS:N    | 2.43                     | 0.47              |
| 53:3:27:G:H2'     | 53:3:28:A:C8     | 2.48                     | 0.47              |
| 53:3:389:A:H3'    | 53:3:390:U:C6    | 2.48                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:3:636:U:H2'   | 53:3:637:C:C6    | 2.48                     | 0.47              |
| 53:3:678:U:H2'   | 53:3:679:C:C6    | 2.49                     | 0.47              |
| 53:3:783:C:O2'   | 53:3:784:A:H5'   | 2.15                     | 0.47              |
| 53:3:1067:A:N3   | 53:3:1068:G:H1'  | 2.30                     | 0.47              |
| 53:3:1091:U:C4   | 53:3:1093:A:C4   | 3.02                     | 0.47              |
| 53:3:1175:G:O2'  | 53:3:1176:A:H5'  | 2.14                     | 0.47              |
| 54:1:296:U:H2'   | 54:1:297:G:H8    | 1.77                     | 0.47              |
| 54:1:1801:A:H5'  | 54:1:1801:A:H8   | 1.78                     | 0.47              |
| 54:1:2314:A:H2'  | 54:1:2315:G:H8   | 1.79                     | 0.47              |
| 54:1:2329:U:H2'  | 54:1:2330:G:H8   | 1.78                     | 0.47              |
| 54:1:2511:U:H2'  | 54:1:2512:C:C6   | 2.48                     | 0.47              |
| 1:b:159:THR:O    | 1:b:194:VAL:HG23 | 2.15                     | 0.47              |
| 2:c:33:ARG:HD3   | 2:c:33:ARG:N     | 2.29                     | 0.47              |
| 2:c:129:THR:HG1  | 54:1:1997:C:C5'  | 2.28                     | 0.47              |
| 2:c:146:ILE:HD11 | 2:c:155:VAL:CG1  | 2.44                     | 0.47              |
| 4:e:35:LEU:CD2   | 4:e:56:LEU:HB3   | 2.44                     | 0.47              |
| 6:g:99:ILE:O     | 6:g:103:VAL:HG23 | 2.15                     | 0.47              |
| 7:h:54:VAL:HG13  | 54:1:1084:A:H5'  | 1.96                     | 0.47              |
| 10:k:24:VAL:CG1  | 10:k:33:ALA:HB2  | 2.39                     | 0.47              |
| 10:k:25:LEU:HD21 | 10:k:40:LYS:HB2  | 1.95                     | 0.47              |
| 22:w:15:LYS:C    | 22:w:17:LEU:HD12 | 2.39                     | 0.47              |
| 22:w:70:PRO:HD3  | 55:2:12:C:H42    | 1.80                     | 0.47              |
| 32:G:17:HIS:HB2  | 32:G:202:ASN:OD1 | 2.14                     | 0.47              |
| 32:G:207:ARG:HD2 | 32:G:208:ALA:N   | 2.29                     | 0.47              |
| 35:J:24:VAL:O    | 35:J:26:GLY:N    | 2.45                     | 0.47              |
| 35:J:40:ASP:CG   | 35:J:44:ARG:HB2  | 2.40                     | 0.47              |
| 35:J:96:GLN:HE21 | 35:J:123:LEU:CG  | 2.27                     | 0.47              |
| 40:O:23:ALA:O    | 40:O:27:GLU:HG3  | 2.14                     | 0.47              |
| 43:R:22:TYR:CD2  | 43:R:65:GLU:HA   | 2.40                     | 0.47              |
| 43:R:97:ARG:HB3  | 53:3:1307:U:N3   | 2.30                     | 0.47              |
| 53:3:834:U:H2'   | 53:3:835:U:C6    | 2.50                     | 0.47              |
| 53:3:859:G:O2'   | 53:3:860:A:H5'   | 2.14                     | 0.47              |
| 53:3:1053:G:O2'  | 53:3:1199:U:C5   | 2.63                     | 0.47              |
| 53:3:1219:A:H2'  | 53:3:1220:G:H8   | 1.79                     | 0.47              |
| 53:3:1238:A:N7   | 53:3:1303:C:H1'  | 2.29                     | 0.47              |
| 53:3:1489:G:H2'  | 53:3:1490:U:C6   | 2.50                     | 0.47              |
| 54:1:493:G:O2'   | 54:1:494:G:H5'   | 2.15                     | 0.47              |
| 54:1:1199:U:H2'  | 54:1:1200:C:H6   | 1.79                     | 0.47              |
| 54:1:1469:A:H2'  | 54:1:1470:A:H8   | 1.80                     | 0.47              |
| 54:1:1924:C:H2'  | 54:1:1925:C:C6   | 2.49                     | 0.47              |
| 54:1:2007:U:H4'  | 54:1:2824:C:H4'  | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:2405:G:H2'   | 54:1:2411:A:N6    | 2.28                     | 0.47              |
| 54:1:2898:U:H2'   | 54:1:2899:A:C8    | 2.50                     | 0.47              |
| 59:8:87:ILE:HD12  | 59:8:87:ILE:H     | 1.79                     | 0.47              |
| 1:b:89:ASN:H      | 1:b:196:ASN:ND2   | 2.11                     | 0.47              |
| 2:c:35:THR:OG1    | 2:c:49:GLN:HG2    | 2.14                     | 0.47              |
| 3:d:48:THR:C      | 3:d:50:ALA:H      | 2.23                     | 0.47              |
| 3:d:149:ILE:HG23  | 3:d:188:MET:HA    | 1.97                     | 0.47              |
| 5:f:51:PHE:HZ     | 5:f:71:LEU:HD22   | 1.78                     | 0.47              |
| 6:g:1:MET:N       | 6:g:20:ASN:OD1    | 2.39                     | 0.47              |
| 13:n:69:ARG:HG3   | 13:n:69:ARG:HH21  | 1.80                     | 0.47              |
| 14:o:4:LYS:HE3    | 14:o:7:ARG:NH2    | 2.30                     | 0.47              |
| 15:p:20:ARG:HD3   | 15:p:112:ARG:CZ   | 2.45                     | 0.47              |
| 29:D:21:ARG:HH21  | 29:D:21:ARG:HG3   | 1.79                     | 0.47              |
| 29:D:26:ASN:CG    | 54:1:682:G:H5'    | 2.39                     | 0.47              |
| 31:F:16:ILE:HD13  | 31:F:25:VAL:HG22  | 1.96                     | 0.47              |
| 32:G:110:ILE:HD13 | 32:G:147:LEU:HD13 | 1.95                     | 0.47              |
| 34:I:150:LYS:NZ   | 34:I:155:LYS:HA   | 2.29                     | 0.47              |
| 35:J:108:GLY:O    | 35:J:109:ALA:HB3  | 2.13                     | 0.47              |
| 37:L:131:GLY:O    | 37:L:134:VAL:HG22 | 2.14                     | 0.47              |
| 38:M:84:ILE:O     | 38:M:123:GLU:OE1  | 2.33                     | 0.47              |
| 38:M:98:LEU:HD12  | 38:M:98:LEU:C     | 2.39                     | 0.47              |
| 40:O:40:ILE:HD11  | 53:3:1124:G:O4'   | 2.15                     | 0.47              |
| 41:P:73:VAL:O     | 41:P:77:GLY:N     | 2.34                     | 0.47              |
| 44:S:24:ALA:O     | 44:S:27:LYS:HG3   | 2.14                     | 0.47              |
| 51:Z:23:GLU:C     | 51:Z:25:ALA:H     | 2.23                     | 0.47              |
| 53:3:349:A:H2'    | 53:3:350:G:O4'    | 2.14                     | 0.47              |
| 53:3:376:G:H2'    | 53:3:377:G:C8     | 2.48                     | 0.47              |
| 53:3:1441:A:C2'   | 53:3:1442:G:H5'   | 2.45                     | 0.47              |
| 54:1:747:C:O2     | 54:1:2014:A:H1'   | 2.15                     | 0.47              |
| 54:1:1429:G:H2'   | 54:1:1430:G:H8    | 1.80                     | 0.47              |
| 54:1:1548:A:H2'   | 54:1:1549:A:C8    | 2.49                     | 0.47              |
| 56:5:29:U:H2'     | 56:5:30:G:H8      | 1.79                     | 0.47              |
| 59:8:315:GLU:HB3  | 59:8:340:SER:OG   | 2.14                     | 0.47              |
| 2:c:116:LYS:HA    | 13:n:1:MET:HE1    | 1.97                     | 0.47              |
| 4:e:129:MET:HA    | 54:1:2304:G:H4'   | 1.96                     | 0.47              |
| 5:f:18:ILE:HG23   | 5:f:18:ILE:O      | 2.14                     | 0.47              |
| 7:h:32:GLY:O      | 54:1:1055:G:H4'   | 2.14                     | 0.47              |
| 8:i:56:VAL:HG21   | 8:i:68:PHE:HD2    | 1.79                     | 0.47              |
| 9:j:27:ARG:NH2    | 54:1:1142:A:H4'   | 2.26                     | 0.47              |
| 12:m:30:SER:O     | 12:m:133:LYS:N    | 2.48                     | 0.47              |
| 14:o:16:ARG:O     | 14:o:19:GLN:HB3   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:q:90:ASP:O     | 16:q:94:LEU:HG    | 2.15                     | 0.47              |
| 18:s:42:LYS:HB2   | 54:1:2010:G:H5'   | 1.97                     | 0.47              |
| 26:A:49:ARG:O     | 49:X:26:ASP:N     | 2.47                     | 0.47              |
| 30:E:23:HIS:ND1   | 30:E:24:LYS:O     | 2.42                     | 0.47              |
| 30:E:24:LYS:HG2   | 30:E:25:HIS:H     | 1.78                     | 0.47              |
| 34:I:27:ILE:HG13  | 34:I:28:ASP:N     | 2.30                     | 0.47              |
| 35:J:24:VAL:CG1   | 35:J:29:ILE:HG13  | 2.45                     | 0.47              |
| 35:J:148:SER:OG   | 35:J:151:MET:HG3  | 2.14                     | 0.47              |
| 36:K:21:MET:HB3   | 36:K:25:TYR:CE2   | 2.49                     | 0.47              |
| 37:L:22:LEU:O     | 37:L:26:VAL:N     | 2.43                     | 0.47              |
| 43:R:97:ARG:N     | 53:3:1307:U:C2'   | 2.63                     | 0.47              |
| 52:a:40:GLU:H     | 52:a:178:VAL:HG22 | 1.78                     | 0.47              |
| 53:3:137:U:H2'    | 53:3:138:G:H8     | 1.79                     | 0.47              |
| 53:3:1127:G:H2'   | 53:3:1128:C:H6    | 1.77                     | 0.47              |
| 53:3:1243:C:H2'   | 53:3:1244:G:H8    | 1.79                     | 0.47              |
| 53:3:1349:A:H1'   | 53:3:1374:A:N6    | 2.30                     | 0.47              |
| 53:3:1501:C:H5'   | 53:3:1502:A:OP2   | 2.14                     | 0.47              |
| 54:1:171:U:H2'    | 54:1:172:A:H8     | 1.80                     | 0.47              |
| 54:1:441:U:O2'    | 54:1:442:G:H5'    | 2.15                     | 0.47              |
| 54:1:494:G:H2'    | 54:1:495:G:H8     | 1.80                     | 0.47              |
| 54:1:898:C:H2'    | 54:1:899:A:O4'    | 2.15                     | 0.47              |
| 54:1:1373:A:C5'   | 54:1:2212:A:H1'   | 2.45                     | 0.47              |
| 54:1:1435:G:O2'   | 54:1:1436:G:H5'   | 2.14                     | 0.47              |
| 54:1:1579:A:H2'   | 54:1:1580:A:H8    | 1.80                     | 0.47              |
| 54:1:1809:A:H2'   | 54:1:1810:A:C8    | 2.49                     | 0.47              |
| 54:1:1838:C:N4    | 54:1:1898:U:H2'   | 2.30                     | 0.47              |
| 54:1:2082:A:H2'   | 54:1:2083:G:O4'   | 2.15                     | 0.47              |
| 54:1:2457:U:O2'   | 54:1:2458:G:H5'   | 2.13                     | 0.47              |
| 54:1:2756:U:H1'   | 54:1:2757:A:H5'   | 1.96                     | 0.47              |
| 57:6:46:G:H3'     | 57:6:47:U:H5'     | 1.97                     | 0.47              |
| 59:8:173:ILE:N    | 59:8:181:GLY:O    | 2.48                     | 0.47              |
| 59:8:572:VAL:HG23 | 59:8:573:ASP:CG   | 2.39                     | 0.47              |
| 1:b:119:VAL:HG11  | 1:b:132:ARG:NH2   | 2.30                     | 0.47              |
| 5:f:89:VAL:HG21   | 5:f:162:ARG:NH1   | 2.28                     | 0.47              |
| 10:k:39:ILE:HG13  | 10:k:41:ILE:HG23  | 1.97                     | 0.47              |
| 20:u:95:PHE:HD2   | 20:u:100:GLU:HB2  | 1.78                     | 0.47              |
| 23:x:39:VAL:O     | 23:x:43:LYS:N     | 2.48                     | 0.47              |
| 26:A:62:LYS:HZ2   | 49:X:17:LYS:HD3   | 1.79                     | 0.47              |
| 29:D:4:THR:HG22   | 54:1:687:C:C1'    | 2.43                     | 0.47              |
| 33:H:52:SER:HB3   | 33:H:114:LEU:HG   | 1.96                     | 0.47              |
| 34:I:12:ARG:HH11  | 34:I:12:ARG:HB3   | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:L:97:ALA:O     | 37:L:101:ARG:HG2  | 2.14                     | 0.47              |
| 38:M:10:LEU:HD22  | 38:M:74:ILE:HD11  | 1.97                     | 0.47              |
| 38:M:114:ALA:O    | 38:M:118:ALA:N    | 2.47                     | 0.47              |
| 52:a:196:LEU:HD13 | 52:a:208:TYR:HE2  | 1.80                     | 0.47              |
| 53:3:231:U:O2'    | 53:3:232:G:H5'    | 2.15                     | 0.47              |
| 53:3:455:G:H2'    | 53:3:456:A:C8     | 2.49                     | 0.47              |
| 53:3:551:U:H2'    | 53:3:552:U:C6     | 2.50                     | 0.47              |
| 53:3:745:G:O2'    | 53:3:746:A:H5'    | 2.15                     | 0.47              |
| 53:3:1074:G:H2'   | 53:3:1075:U:H6    | 1.80                     | 0.47              |
| 53:3:1345:U:H2'   | 53:3:1377:A:N1    | 2.30                     | 0.47              |
| 54:1:1468:U:H2'   | 54:1:1522:A:N6    | 2.29                     | 0.47              |
| 54:1:1786:A:H1'   | 54:1:1938:A:H61   | 1.79                     | 0.47              |
| 59:8:353:VAL:HG11 | 59:8:395:ASP:CB   | 2.45                     | 0.47              |
| 59:8:496:GLN:CG   | 59:8:608:ALA:HA   | 2.45                     | 0.47              |
| 1:b:28:PRO:HB2    | 1:b:33:LEU:HD11   | 1.97                     | 0.47              |
| 2:c:9:VAL:HA      | 2:c:197:THR:HG23  | 1.96                     | 0.47              |
| 2:c:51:THR:OG1    | 2:c:76:GLY:HA3    | 2.14                     | 0.47              |
| 7:h:61:ARG:HH11   | 7:h:61:ARG:HG3    | 1.79                     | 0.47              |
| 15:p:50:ARG:HH12  | 15:p:52:ARG:HG3   | 1.79                     | 0.47              |
| 17:r:68:ARG:HB2   | 17:r:90:ARG:NH2   | 2.30                     | 0.47              |
| 24:y:48:ARG:HG3   | 24:y:48:ARG:HH11  | 1.80                     | 0.47              |
| 32:G:43:GLU:CD    | 32:G:43:GLU:H     | 2.23                     | 0.47              |
| 32:G:44:LYS:C     | 32:G:47:PRO:HD2   | 2.39                     | 0.47              |
| 32:G:68:PHE:HD2   | 32:G:83:ALA:HB2   | 1.80                     | 0.47              |
| 32:G:100:LEU:HB2  | 32:G:174:GLU:OE2  | 2.15                     | 0.47              |
| 32:G:198:VAL:C    | 32:G:199:ILE:HD12 | 2.39                     | 0.47              |
| 35:J:107:GLY:HA3  | 53:3:9:G:H5'      | 1.97                     | 0.47              |
| 36:K:8:PHE:HB2    | 36:K:87:SER:OG    | 2.15                     | 0.47              |
| 36:K:47:LEU:HG    | 36:K:55:HIS:O     | 2.15                     | 0.47              |
| 44:S:53:ASP:O     | 44:S:55:SER:N     | 2.47                     | 0.47              |
| 46:U:20:VAL:HG23  | 46:U:35:ARG:HA    | 1.97                     | 0.47              |
| 51:Z:28:LEU:HD23  | 51:Z:28:LEU:C     | 2.40                     | 0.47              |
| 53:3:66:A:O2'     | 53:3:67:C:H5'     | 2.15                     | 0.47              |
| 53:3:243:A:H4'    | 53:3:244:U:H3'    | 1.97                     | 0.47              |
| 53:3:955:U:H3     | 53:3:1225:A:N6    | 2.12                     | 0.47              |
| 53:3:986:U:O4     | 53:3:1219:A:N1    | 2.47                     | 0.47              |
| 53:3:1004:A:H2'   | 53:3:1005:A:O4'   | 2.15                     | 0.47              |
| 53:3:1012:A:H8    | 53:3:1012:A:O5'   | 1.97                     | 0.47              |
| 53:3:1283:U:H2'   | 53:3:1284:C:C6    | 2.50                     | 0.47              |
| 53:3:1488:G:O2'   | 53:3:1489:G:H5'   | 2.15                     | 0.47              |
| 54:1:638:G:H2'    | 54:1:639:U:C6     | 2.50                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:1171:G:H1    | 54:1:1178:C:H42   | 1.63                     | 0.47              |
| 54:1:1726:C:H2'   | 54:1:1727:C:H6    | 1.80                     | 0.47              |
| 54:1:1866:A:H2'   | 54:1:1867:G:O4'   | 2.15                     | 0.47              |
| 54:1:1880:U:H2'   | 54:1:1881:C:C6    | 2.49                     | 0.47              |
| 59:8:101:ARG:HH21 | 59:8:393:THR:HG21 | 1.80                     | 0.47              |
| 59:8:125:THR:O    | 59:8:128:ARG:N    | 2.48                     | 0.47              |
| 59:8:475:ARG:HH11 | 59:8:475:ARG:CA   | 2.27                     | 0.47              |
| 59:8:621:VAL:HG12 | 59:8:680:TYR:CB   | 2.44                     | 0.47              |
| 59:8:623:THR:HG21 | 59:8:631:VAL:HG21 | 1.97                     | 0.47              |
| 3:d:192:ALA:O     | 3:d:196:VAL:HG23  | 2.15                     | 0.47              |
| 6:g:121:VAL:HG23  | 6:g:123:ARG:HG3   | 1.96                     | 0.47              |
| 9:j:48:VAL:HG23   | 9:j:50:THR:HG23   | 1.97                     | 0.47              |
| 9:j:99:ARG:NH2    | 9:j:103:ILE:HD11  | 2.30                     | 0.47              |
| 12:m:74:THR:HG21  | 12:m:86:LYS:HE2   | 1.97                     | 0.47              |
| 13:n:35:LYS:HE2   | 13:n:110:MET:HG2  | 1.97                     | 0.47              |
| 17:r:74:ILE:HB    | 17:r:87:GLN:NE2   | 2.30                     | 0.47              |
| 20:u:95:PHE:CE2   | 20:u:102:ILE:HG12 | 2.49                     | 0.47              |
| 21:v:75:GLN:HB2   | 21:v:92:VAL:H     | 1.80                     | 0.47              |
| 34:l:183:ARG:H    | 34:l:183:ARG:CD   | 2.27                     | 0.47              |
| 40:O:7:ARG:O      | 40:O:101:SER:N    | 2.40                     | 0.47              |
| 40:O:84:VAL:HA    | 40:O:87:LEU:HD12  | 1.97                     | 0.47              |
| 44:S:8:ARG:NE     | 53:3:1217:C:OP1   | 2.48                     | 0.47              |
| 49:X:18:VAL:HG11  | 49:X:43:MET:HG3   | 1.96                     | 0.47              |
| 51:Z:36:PHE:C     | 51:Z:38:GLU:H     | 2.22                     | 0.47              |
| 53:3:490:C:H2'    | 53:3:491:G:C8     | 2.50                     | 0.47              |
| 53:3:1069:C:H2'   | 53:3:1070:U:H5'   | 1.97                     | 0.47              |
| 54:1:1780:A:H3'   | 54:1:1781:U:H2'   | 1.97                     | 0.47              |
| 56:5:29:U:H2'     | 56:5:30:G:C8      | 2.50                     | 0.47              |
| 59:8:276:GLN:NE2  | 59:8:280:ASP:OD2  | 2.48                     | 0.47              |
| 59:8:419:ALA:O    | 59:8:484:GLY:N    | 2.47                     | 0.47              |
| 1:b:224:MET:O     | 1:b:232:GLY:HA2   | 2.15                     | 0.46              |
| 3:d:38:GLY:HA3    | 54:1:615:U:O2     | 2.15                     | 0.46              |
| 3:d:149:ILE:HG23  | 3:d:149:ILE:O     | 2.15                     | 0.46              |
| 5:f:59:ASP:OD2    | 5:f:63:GLN:HG2    | 2.14                     | 0.46              |
| 15:p:88:ARG:HH11  | 15:p:113:LEU:HA   | 1.80                     | 0.46              |
| 23:x:14:GLY:O     | 23:x:26:ARG:N     | 2.48                     | 0.46              |
| 26:A:56:ARG:O     | 26:A:60:PHE:N     | 2.41                     | 0.46              |
| 30:E:13:PHE:C     | 30:E:14:LYS:HD2   | 2.40                     | 0.46              |
| 32:G:150:ILE:HA   | 32:G:153:MET:HB3  | 1.97                     | 0.46              |
| 33:H:148:ILE:HG12 | 33:H:149:LYS:N    | 2.30                     | 0.46              |
| 35:J:59:ILE:O     | 35:J:63:MET:HG2   | 2.14                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 36:K:11:HIS:CE1  | 36:K:54:LEU:HD13 | 2.50                     | 0.46              |
| 37:L:25:PHE:HD1  | 37:L:100:MET:HB3 | 1.79                     | 0.46              |
| 39:N:78:ILE:O    | 39:N:82:ILE:HG12 | 2.15                     | 0.46              |
| 40:O:88:MET:HE2  | 40:O:88:MET:HA   | 1.97                     | 0.46              |
| 41:P:92:ARG:HH22 | 41:P:111:ASP:CG  | 2.23                     | 0.46              |
| 41:P:123:PRO:HG2 | 51:Z:33:ARG:CB   | 2.45                     | 0.46              |
| 42:Q:35:ARG:HG3  | 42:Q:37:TYR:CD1  | 2.51                     | 0.46              |
| 42:Q:86:VAL:C    | 42:Q:88:ASP:H    | 2.24                     | 0.46              |
| 45:T:35:ILE:HD12 | 45:T:62:ARG:NH1  | 2.29                     | 0.46              |
| 45:T:53:ARG:HH21 | 53:3:579:A:H4'   | 1.80                     | 0.46              |
| 53:3:531:U:H4'   | 53:3:532:A:C5'   | 2.39                     | 0.46              |
| 53:3:677:U:H2'   | 53:3:678:U:H6    | 1.79                     | 0.46              |
| 53:3:728:A:H2'   | 53:3:729:A:C8    | 2.50                     | 0.46              |
| 53:3:818:G:H3'   | 53:3:819:A:C5'   | 2.45                     | 0.46              |
| 53:3:921:U:H4'   | 53:3:1082:A:OP1  | 2.14                     | 0.46              |
| 53:3:990:C:H2'   | 53:3:991:U:C1'   | 2.45                     | 0.46              |
| 53:3:1046:A:H2'  | 53:3:1047:G:O4'  | 2.16                     | 0.46              |
| 53:3:1168:U:H3'  | 53:3:1168:U:O2   | 2.15                     | 0.46              |
| 53:3:1258:G:H2'  | 53:3:1259:C:C6   | 2.50                     | 0.46              |
| 53:3:1386:G:O2'  | 53:3:1387:G:H5'  | 2.15                     | 0.46              |
| 54:1:893:C:H2'   | 54:1:894:U:C6    | 2.50                     | 0.46              |
| 54:1:1542:U:H2'  | 54:1:1543:G:O4'  | 2.16                     | 0.46              |
| 54:1:1810:A:C2'  | 54:1:1811:G:H5'  | 2.44                     | 0.46              |
| 54:1:2024:G:H2'  | 54:1:2025:C:C6   | 2.50                     | 0.46              |
| 54:1:2104:C:H2'  | 54:1:2105:U:H6   | 1.79                     | 0.46              |
| 54:1:2648:G:H2'  | 54:1:2649:C:C6   | 2.50                     | 0.46              |
| 54:1:2715:C:C3'  | 54:1:2716:C:H5'' | 2.45                     | 0.46              |
| 54:1:2750:A:N3   | 54:1:2752:C:N4   | 2.63                     | 0.46              |
| 54:1:2756:U:H4'  | 54:1:2757:A:OP1  | 2.15                     | 0.46              |
| 4:e:63:LYS:HB2   | 26:A:5:ILE:O     | 2.16                     | 0.46              |
| 4:e:108:PRO:HG3  | 26:A:38:SER:HB3  | 1.98                     | 0.46              |
| 4:e:166:ARG:CB   | 4:e:166:ARG:NH1  | 2.78                     | 0.46              |
| 7:h:77:VAL:O     | 7:h:77:VAL:HG22  | 2.15                     | 0.46              |
| 8:i:9:LYS:O      | 8:i:10:LEU:HD23  | 2.14                     | 0.46              |
| 11:l:29:LYS:C    | 11:l:30:THR:HG23 | 2.40                     | 0.46              |
| 11:l:90:VAL:HG13 | 11:l:95:LEU:HD21 | 1.97                     | 0.46              |
| 18:s:40:ASN:O    | 18:s:41:LYS:HD2  | 2.15                     | 0.46              |
| 24:y:23:ARG:HG2  | 24:y:24:GLU:N    | 2.29                     | 0.46              |
| 25:z:4:ILE:N     | 25:z:37:ARG:O    | 2.48                     | 0.46              |
| 34:I:96:ARG:HH11 | 34:I:96:ARG:HG3  | 1.80                     | 0.46              |
| 34:I:97:LEU:HG   | 34:I:134:TYR:HB3 | 1.97                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 35:J:13:LYS:HD3   | 35:J:112:ALA:HA  | 1.97                     | 0.46              |
| 36:K:17:GLN:C     | 36:K:19:PRO:HD2  | 2.40                     | 0.46              |
| 36:K:91:ARG:HD3   | 53:3:738:C:P     | 2.55                     | 0.46              |
| 42:Q:19:ASN:HD22  | 42:Q:19:ASN:C    | 2.21                     | 0.46              |
| 43:R:102:LYS:O    | 43:R:102:LYS:HG2 | 2.15                     | 0.46              |
| 47:V:62:GLU:HG2   | 47:V:63:CYS:N    | 2.30                     | 0.46              |
| 50:Y:60:GLN:HA    | 50:Y:63:LYS:HB2  | 1.96                     | 0.46              |
| 53:3:1314:C:H6    | 53:3:1314:C:O5'  | 1.97                     | 0.46              |
| 53:3:1509:C:O2'   | 53:3:1510:C:H5'  | 2.15                     | 0.46              |
| 54:1:971:G:H2'    | 54:1:972:A:O4'   | 2.15                     | 0.46              |
| 54:1:1053:C:H2'   | 54:1:1054:A:H5'' | 1.97                     | 0.46              |
| 54:1:1475:G:O2'   | 54:1:1476:U:C6   | 2.67                     | 0.46              |
| 54:1:2179:C:H2'   | 54:1:2180:U:H6   | 1.78                     | 0.46              |
| 54:1:2314:A:H2'   | 54:1:2315:G:C8   | 2.50                     | 0.46              |
| 59:8:263:LEU:HD13 | 59:8:281:ALA:HB1 | 1.97                     | 0.46              |
| 59:8:326:THR:HA   | 59:8:332:ASN:HA  | 1.96                     | 0.46              |
| 59:8:466:LEU:HD12 | 59:8:466:LEU:N   | 2.30                     | 0.46              |
| 2:c:194:PRO:HA    | 54:1:2680:U:H5'  | 1.96                     | 0.46              |
| 5:f:3:VAL:HG21    | 54:1:2748:A:H5'  | 1.98                     | 0.46              |
| 13:n:9:GLN:HG3    | 13:n:17:ARG:HH22 | 1.80                     | 0.46              |
| 15:p:21:PRO:HB3   | 15:p:49:ILE:CD1  | 2.45                     | 0.46              |
| 16:q:93:ILE:O     | 16:q:97:ILE:HG13 | 2.14                     | 0.46              |
| 25:z:4:ILE:HG22   | 25:z:37:ARG:O    | 2.15                     | 0.46              |
| 32:G:39:ILE:HG22  | 32:G:40:ILE:O    | 2.15                     | 0.46              |
| 32:G:40:ILE:HG22  | 32:G:41:ASN:N    | 2.31                     | 0.46              |
| 32:G:163:ILE:O    | 32:G:185:ILE:HB  | 2.16                     | 0.46              |
| 36:K:3:HIS:CD2    | 36:K:95:ALA:HB2  | 2.50                     | 0.46              |
| 38:M:98:LEU:HD12  | 38:M:99:GLY:N    | 2.31                     | 0.46              |
| 39:N:98:ARG:HH22  | 53:3:1180:A:P    | 2.37                     | 0.46              |
| 40:O:18:ILE:HG23  | 40:O:72:ARG:HH12 | 1.79                     | 0.46              |
| 41:P:15:VAL:HG12  | 41:P:76:TYR:HB3  | 1.97                     | 0.46              |
| 42:Q:28:GLN:HB3   | 42:Q:80:LEU:HG   | 1.97                     | 0.46              |
| 44:S:86:ALA:HB1   | 44:S:91:GLU:HB2  | 1.96                     | 0.46              |
| 46:U:5:ARG:HB2    | 53:3:376:G:H5''  | 1.97                     | 0.46              |
| 53:3:477:C:H2'    | 53:3:478:A:H8    | 1.78                     | 0.46              |
| 53:3:765:G:C5     | 53:3:812:G:C2    | 3.03                     | 0.46              |
| 54:1:163:C:H2'    | 54:1:164:C:O4'   | 2.15                     | 0.46              |
| 54:1:455:C:O2     | 54:1:472:A:H2'   | 2.16                     | 0.46              |
| 54:1:893:C:O2'    | 54:1:894:U:H5'   | 2.15                     | 0.46              |
| 54:1:1070:A:H2'   | 54:1:1097:U:OP1  | 2.14                     | 0.46              |
| 54:1:2691:C:O2'   | 54:1:2692:G:H5'  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:2802:G:H2'   | 54:1:2803:G:C8    | 2.51                     | 0.46              |
| 59:8:97:ILE:HG12  | 59:8:443:PRO:HG2  | 1.97                     | 0.46              |
| 59:8:146:ARG:O    | 59:8:176:GLU:HG2  | 2.15                     | 0.46              |
| 59:8:158:ILE:CD1  | 59:8:162:LEU:HD12 | 2.44                     | 0.46              |
| 3:d:148:ILE:N     | 3:d:168:ASP:O     | 2.47                     | 0.46              |
| 7:h:41:LEU:HA     | 7:h:44:ALA:HB3    | 1.96                     | 0.46              |
| 13:n:64:ARG:HH21  | 13:n:64:ARG:HG3   | 1.81                     | 0.46              |
| 21:v:63:ILE:CG2   | 21:v:70:ILE:HB    | 2.41                     | 0.46              |
| 25:z:36:GLU:O     | 25:z:37:ARG:NH1   | 2.48                     | 0.46              |
| 40:O:56:HIS:CE1   | 53:3:963:G:H21    | 2.33                     | 0.46              |
| 44:S:15:LEU:HD23  | 44:S:15:LEU:C     | 2.41                     | 0.46              |
| 51:Z:39:LYS:O     | 51:Z:43:GLU:N     | 2.35                     | 0.46              |
| 53:3:1114:C:C2    | 53:3:1115:U:N3    | 2.83                     | 0.46              |
| 53:3:1138:G:H3'   | 53:3:1138:G:N3    | 2.31                     | 0.46              |
| 53:3:1200:C:C4'   | 53:3:1201:A:H3'   | 2.46                     | 0.46              |
| 54:1:481:G:H1'    | 54:1:506:G:H21    | 1.76                     | 0.46              |
| 54:1:2533:U:H2'   | 54:1:2534:A:C5'   | 2.46                     | 0.46              |
| 54:1:2660:A:N7    | 59:8:672:SER:HA   | 2.30                     | 0.46              |
| 55:2:66:A:N1      | 55:2:107:G:H2'    | 2.31                     | 0.46              |
| 2:c:135:GLY:HA2   | 54:1:743:A:OP1    | 2.16                     | 0.46              |
| 3:d:30:GLN:CD     | 54:1:659:G:H21    | 2.23                     | 0.46              |
| 9:j:32:LEU:HB3    | 9:j:36:LEU:HD23   | 1.98                     | 0.46              |
| 9:j:80:HIS:CD2    | 54:1:2642:G:H5''  | 2.50                     | 0.46              |
| 15:p:47:ILE:HG13  | 15:p:59:THR:OG1   | 2.15                     | 0.46              |
| 15:p:87:ARG:HH21  | 15:p:111:GLU:HG3  | 1.81                     | 0.46              |
| 26:A:62:LYS:NZ    | 49:X:17:LYS:HA    | 2.31                     | 0.46              |
| 40:O:7:ARG:HE     | 40:O:75:ASP:CG    | 2.24                     | 0.46              |
| 40:O:53:ILE:CG1   | 53:3:1060:U:H5''  | 2.45                     | 0.46              |
| 44:S:99:SER:HB2   | 53:3:1187:G:H21   | 1.80                     | 0.46              |
| 47:V:59:GLU:HG3   | 47:V:76:ARG:CZ    | 2.45                     | 0.46              |
| 50:Y:66:ILE:CG2   | 50:Y:67:HIS:N     | 2.78                     | 0.46              |
| 53:3:225:C:C3'    | 53:3:226:G:H5''   | 2.46                     | 0.46              |
| 53:3:571:U:C3'    | 53:3:572:A:H5''   | 2.46                     | 0.46              |
| 53:3:866:C:C4'    | 53:3:919:A:H5'    | 2.34                     | 0.46              |
| 53:3:1008:U:H2'   | 53:3:1009:U:O4'   | 2.15                     | 0.46              |
| 54:1:689:A:H2'    | 54:1:690:G:H8     | 1.80                     | 0.46              |
| 54:1:1066:U:H3'   | 54:1:1067:A:C5'   | 2.46                     | 0.46              |
| 54:1:1443:U:H2'   | 54:1:1444:G:C8    | 2.51                     | 0.46              |
| 54:1:2662:A:H5'   | 59:8:464:LEU:HD21 | 1.97                     | 0.46              |
| 59:8:374:ILE:HG22 | 59:8:375:LYS:N    | 2.31                     | 0.46              |
| 1:b:42:ARG:HH12   | 54:1:690:G:H21    | 1.63                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:e:55:ASP:O      | 4:e:59:ILE:HG13   | 2.15                     | 0.46              |
| 32:G:22:TRP:N     | 32:G:22:TRP:CD1   | 2.83                     | 0.46              |
| 32:G:108:GLN:O    | 32:G:111:LYS:HB3  | 2.16                     | 0.46              |
| 32:G:148:GLY:O    | 32:G:151:LYS:HB3  | 2.15                     | 0.46              |
| 32:G:160:LEU:HD23 | 32:G:182:VAL:HG12 | 1.97                     | 0.46              |
| 33:H:118:SER:O    | 33:H:122:GLN:HG2  | 2.16                     | 0.46              |
| 33:H:137:VAL:HG11 | 33:H:167:TYR:CE2  | 2.51                     | 0.46              |
| 35:J:114:LEU:HD12 | 35:J:119:VAL:HG21 | 1.98                     | 0.46              |
| 36:K:15:SER:HB2   | 36:K:58:HIS:HB2   | 1.97                     | 0.46              |
| 38:M:5:PRO:HA     | 38:M:8:ASP:HB3    | 1.98                     | 0.46              |
| 39:N:20:ILE:HG13  | 39:N:62:LEU:HG    | 1.97                     | 0.46              |
| 41:P:92:ARG:HH11  | 41:P:92:ARG:HG3   | 1.80                     | 0.46              |
| 45:T:24:THR:HG21  | 45:T:69:LEU:HD22  | 1.98                     | 0.46              |
| 50:Y:66:ILE:C     | 50:Y:68:LYS:H     | 2.24                     | 0.46              |
| 53:3:16:A:C2      | 53:3:1080:A:C8    | 3.04                     | 0.46              |
| 53:3:156:C:O2'    | 53:3:157:U:H5'    | 2.15                     | 0.46              |
| 53:3:714:G:H2'    | 53:3:715:A:H8     | 1.78                     | 0.46              |
| 53:3:1059:C:H2'   | 53:3:1060:U:C6    | 2.51                     | 0.46              |
| 53:3:1210:C:H2'   | 53:3:1211:U:H5'   | 1.98                     | 0.46              |
| 54:1:17:G:H2'     | 54:1:18:U:H6      | 1.77                     | 0.46              |
| 54:1:837:C:O2'    | 54:1:838:C:H5'    | 2.16                     | 0.46              |
| 54:1:1163:G:O2'   | 54:1:1164:C:H5'   | 2.16                     | 0.46              |
| 54:1:1516:G:O2'   | 54:1:1517:G:H5'   | 2.16                     | 0.46              |
| 54:1:2039:U:H2'   | 54:1:2040:G:H8    | 1.81                     | 0.46              |
| 54:1:2108:A:C2'   | 54:1:2109:U:H5'   | 2.46                     | 0.46              |
| 54:1:2715:C:H2'   | 54:1:2716:C:H5''  | 1.97                     | 0.46              |
| 54:1:2861:U:H2'   | 54:1:2862:G:C8    | 2.49                     | 0.46              |
| 59:8:13:ILE:HG13  | 59:8:86:ILE:HD13  | 1.98                     | 0.46              |
| 59:8:104:ARG:HG2  | 59:8:104:ARG:HH11 | 1.80                     | 0.46              |
| 59:8:168:PRO:C    | 59:8:170:GLN:N    | 2.74                     | 0.46              |
| 59:8:173:ILE:HG12 | 59:8:211:MET:HE1  | 1.97                     | 0.46              |
| 59:8:349:VAL:HG12 | 59:8:399:ASP:HB3  | 1.96                     | 0.46              |
| 1:b:73:ILE:HG23   | 54:1:1490:A:N6    | 2.31                     | 0.46              |
| 3:d:188:MET:CE    | 3:d:193:VAL:HG22  | 2.43                     | 0.46              |
| 4:e:101:ARG:HG3   | 4:e:101:ARG:NH2   | 2.31                     | 0.46              |
| 5:f:15:ASP:HB3    | 5:f:26:LYS:HB3    | 1.98                     | 0.46              |
| 9:j:116:ARG:O     | 9:j:119:PHE:HB3   | 2.15                     | 0.46              |
| 15:p:113:LEU:HD21 | 53:3:1441:A:N1    | 2.30                     | 0.46              |
| 18:s:4:ILE:O      | 18:s:4:ILE:HG23   | 2.16                     | 0.46              |
| 40:O:7:ARG:HD3    | 40:O:73:LEU:HD21  | 1.96                     | 0.46              |
| 43:R:100:ARG:HB3  | 53:3:949:A:OP1    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:V:13:SER:HB3   | 47:V:21:VAL:CG1   | 2.46                     | 0.46              |
| 50:Y:54:GLN:N     | 50:Y:55:PRO:HD2   | 2.30                     | 0.46              |
| 53:3:236:A:H2'    | 53:3:237:G:C8     | 2.51                     | 0.46              |
| 53:3:483:C:H3'    | 53:3:484:G:H2'    | 1.97                     | 0.46              |
| 53:3:632:U:H3'    | 53:3:633:G:H5'    | 1.98                     | 0.46              |
| 53:3:919:A:C2'    | 53:3:920:U:O5'    | 2.63                     | 0.46              |
| 54:1:127:A:H5''   | 54:1:128:C:O4'    | 2.16                     | 0.46              |
| 54:1:171:U:H2'    | 54:1:172:A:C8     | 2.51                     | 0.46              |
| 54:1:549:G:H2'    | 54:1:550:C:C6     | 2.50                     | 0.46              |
| 54:1:828:U:H4'    | 54:1:831:G:C2     | 2.51                     | 0.46              |
| 54:1:1802:A:H2'   | 54:1:1803:A:H8    | 1.80                     | 0.46              |
| 54:1:2814:A:H2'   | 54:1:2815:C:C6    | 2.51                     | 0.46              |
| 55:2:30:C:H2'     | 55:2:31:C:O4'     | 2.16                     | 0.46              |
| 59:8:10:TYR:HE1   | 59:8:83:ARG:HE    | 1.62                     | 0.46              |
| 59:8:102:SER:O    | 59:8:106:LEU:HG   | 2.15                     | 0.46              |
| 59:8:295:ILE:HG21 | 59:8:309:ARG:HH21 | 1.81                     | 0.46              |
| 59:8:310:HIS:HB2  | 59:8:315:GLU:HG2  | 1.98                     | 0.46              |
| 8:i:25:PRO:HD2    | 59:8:645:GLN:NE2  | 2.31                     | 0.46              |
| 8:i:41:PHE:CE1    | 8:i:45:THR:HG21   | 2.51                     | 0.46              |
| 9:j:27:ARG:HH11   | 9:j:27:ARG:HG3    | 1.81                     | 0.46              |
| 34:I:3:TYR:O      | 34:I:4:LEU:HD12   | 2.15                     | 0.46              |
| 34:I:57:LYS:HD2   | 34:I:57:LYS:C     | 2.40                     | 0.46              |
| 34:I:201:GLU:O    | 53:3:8:A:N6       | 2.46                     | 0.46              |
| 37:L:16:LYS:HD2   | 37:L:17:PHE:HE1   | 1.80                     | 0.46              |
| 43:R:99:GLN:CG    | 43:R:100:ARG:H    | 2.23                     | 0.46              |
| 44:S:58:ARG:HE    | 44:S:58:ARG:HB3   | 1.59                     | 0.46              |
| 49:X:42:ASN:ND2   | 49:X:43:MET:SD    | 2.88                     | 0.46              |
| 50:Y:8:LYS:O      | 50:Y:11:ILE:HG12  | 2.16                     | 0.46              |
| 53:3:16:A:N1      | 53:3:17:U:C5      | 2.84                     | 0.46              |
| 53:3:26:A:H61     | 53:3:558:G:H1'    | 1.81                     | 0.46              |
| 53:3:584:G:H2'    | 53:3:585:G:H8     | 1.81                     | 0.46              |
| 53:3:711:G:O2'    | 53:3:712:A:H5'    | 2.16                     | 0.46              |
| 53:3:1127:G:H2'   | 53:3:1128:C:C6    | 2.51                     | 0.46              |
| 53:3:1144:G:O2'   | 53:3:1145:A:H5'   | 2.16                     | 0.46              |
| 53:3:1175:G:H2'   | 53:3:1176:A:O4'   | 2.16                     | 0.46              |
| 54:1:964:C:O2     | 54:1:2273:A:H2    | 1.98                     | 0.46              |
| 54:1:1084:A:H2'   | 54:1:1105:U:O2'   | 2.15                     | 0.46              |
| 54:1:1750:G:H2'   | 54:1:1751:U:C6    | 2.51                     | 0.46              |
| 54:1:2081:U:H2'   | 54:1:2082:A:C8    | 2.51                     | 0.46              |
| 54:1:2557:G:H2'   | 54:1:2558:C:H6    | 1.81                     | 0.46              |
| 56:5:36:G:O2'     | 59:8:508:GLN:HB3  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 56:5:49:G:H1      | 56:5:65:U:H3      | 1.62                     | 0.46              |
| 59:8:263:LEU:HD11 | 59:8:285:TYR:HB2  | 1.97                     | 0.46              |
| 59:8:360:PHE:HB3  | 59:8:363:ILE:HD11 | 1.98                     | 0.46              |
| 59:8:495:ARG:HH11 | 59:8:495:ARG:HG3  | 1.80                     | 0.46              |
| 4:e:42:ALA:HB2    | 4:e:48:LEU:HD22   | 1.98                     | 0.46              |
| 5:f:175:LYS:O     | 5:f:176:LYS:HD3   | 2.15                     | 0.46              |
| 7:h:34:THR:O      | 7:h:37:LYS:HB3    | 2.16                     | 0.46              |
| 10:k:63:VAL:HG12  | 10:k:107:LEU:HD22 | 1.98                     | 0.46              |
| 11:l:16:GLY:HA2   | 54:1:662:G:O3'    | 2.16                     | 0.46              |
| 11:l:23:ILE:HD13  | 17:r:84:ARG:NH1   | 2.31                     | 0.46              |
| 11:l:50:PHE:CE2   | 11:l:52:GLY:HA2   | 2.51                     | 0.46              |
| 11:l:95:LEU:HB3   | 11:l:100:ILE:HG12 | 1.97                     | 0.46              |
| 24:y:23:ARG:HD3   | 24:y:23:ARG:N     | 2.30                     | 0.46              |
| 31:F:17:VAL:CG1   | 31:F:19:ARG:HG3   | 2.45                     | 0.46              |
| 32:G:110:ILE:CD1  | 32:G:147:LEU:HD13 | 2.46                     | 0.46              |
| 35:J:160:VAL:O    | 35:J:164:LEU:HG   | 2.16                     | 0.46              |
| 39:N:5:TYR:HB2    | 39:N:20:ILE:CG2   | 2.45                     | 0.46              |
| 47:V:11:VAL:CG2   | 47:V:20:ILE:HD11  | 2.45                     | 0.46              |
| 47:V:74:LEU:HD12  | 47:V:75:VAL:H     | 1.80                     | 0.46              |
| 50:Y:43:LYS:HB3   | 50:Y:85:LEU:HD22  | 1.96                     | 0.46              |
| 54:1:69:C:H2'     | 54:1:70:G:C8      | 2.51                     | 0.46              |
| 54:1:296:U:H2'    | 54:1:297:G:C8     | 2.51                     | 0.46              |
| 54:1:483:A:H3'    | 54:1:484:C:H6     | 1.81                     | 0.46              |
| 54:1:665:U:H2'    | 54:1:666:A:H8     | 1.81                     | 0.46              |
| 54:1:2123:G:H2'   | 54:1:2124:G:C8    | 2.51                     | 0.46              |
| 54:1:2590:A:O2'   | 54:1:2591:C:H5'   | 2.15                     | 0.46              |
| 59:8:220:GLN:O    | 59:8:224:GLU:HB2  | 2.16                     | 0.46              |
| 3:d:71:GLY:N      | 54:1:674:G:H5''   | 2.31                     | 0.46              |
| 8:i:34:ILE:HG23   | 8:i:35:MET:N      | 2.31                     | 0.46              |
| 9:j:47:HIS:CD2    | 54:1:536:G:H21    | 2.34                     | 0.46              |
| 11:l:93:ASN:C     | 11:l:95:LEU:N     | 2.73                     | 0.46              |
| 15:p:30:TRP:CE3   | 15:p:30:TRP:HA    | 2.50                     | 0.46              |
| 18:s:24:ILE:HD11  | 18:s:47:VAL:HG21  | 1.99                     | 0.46              |
| 26:A:11:GLU:HB2   | 26:A:25:ARG:HH11  | 1.81                     | 0.46              |
| 29:D:35:ARG:NH1   | 29:D:35:ARG:CB    | 2.79                     | 0.46              |
| 30:E:53:ASP:HB3   | 30:E:56:LEU:HD12  | 1.98                     | 0.46              |
| 33:H:130:ARG:HA   | 33:H:133:MET:HG2  | 1.98                     | 0.46              |
| 35:J:80:LEU:HD13  | 35:J:122:VAL:HG11 | 1.98                     | 0.46              |
| 35:J:160:VAL:HG13 | 35:J:161:GLU:N    | 2.31                     | 0.46              |
| 38:M:42:GLU:HG2   | 38:M:100:ILE:HD13 | 1.96                     | 0.46              |
| 38:M:73:SER:HB3   | 38:M:129:ALA:HB3  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:333:U:H2'    | 53:3:334:C:C6     | 2.51                     | 0.46              |
| 53:3:922:G:H2'    | 53:3:923:A:O4'    | 2.16                     | 0.46              |
| 53:3:1157:A:N6    | 53:3:1178:G:H1'   | 2.31                     | 0.46              |
| 53:3:1306:A:N6    | 53:3:1331:G:O2'   | 2.49                     | 0.46              |
| 53:3:1329:A:H2'   | 53:3:1330:U:O4'   | 2.16                     | 0.46              |
| 54:1:1680:U:H2'   | 54:1:1681:G:O4'   | 2.16                     | 0.46              |
| 54:1:2070:A:H2'   | 54:1:2071:A:O4'   | 2.16                     | 0.46              |
| 54:1:2282:G:H1'   | 54:1:2390:U:H3    | 1.81                     | 0.46              |
| 54:1:2497:A:H8    | 54:1:2497:A:OP2   | 1.98                     | 0.46              |
| 55:2:29:A:H2'     | 55:2:30:C:H6      | 1.80                     | 0.46              |
| 56:5:24:G:H2'     | 56:5:25:C:C6      | 2.51                     | 0.46              |
| 59:8:123:SER:O    | 59:8:126:VAL:HG22 | 2.15                     | 0.46              |
| 59:8:342:VAL:HA   | 59:8:377:VAL:O    | 2.15                     | 0.46              |
| 4:e:84:ILE:HG21   | 54:1:2312:U:H4'   | 1.97                     | 0.45              |
| 4:e:175:PRO:O     | 26:A:47:LYS:NZ    | 2.48                     | 0.45              |
| 11:l:55:MET:HE3   | 54:1:2392:A:C2    | 2.50                     | 0.45              |
| 20:u:73:ASN:C     | 20:u:75:ALA:H     | 2.24                     | 0.45              |
| 22:w:56:PHE:CE2   | 54:1:2365:G:H4'   | 2.50                     | 0.45              |
| 26:A:44:PHE:H     | 26:A:44:PHE:HD1   | 1.62                     | 0.45              |
| 30:E:30:HIS:CE1   | 30:E:31:ILE:HG12  | 2.50                     | 0.45              |
| 31:F:23:ILE:H     | 31:F:23:ILE:CD1   | 2.20                     | 0.45              |
| 33:H:110:LEU:HD13 | 33:H:203:LYS:HZ1  | 1.81                     | 0.45              |
| 33:H:129:PHE:HD1  | 33:H:129:PHE:H    | 1.62                     | 0.45              |
| 37:L:73:GLU:CG    | 37:L:74:VAL:H     | 2.25                     | 0.45              |
| 37:L:92:PRO:HA    | 37:L:95:ARG:CB    | 2.45                     | 0.45              |
| 38:M:9:MET:CB     | 38:M:26:MET:HE1   | 2.46                     | 0.45              |
| 40:O:53:ILE:HG13  | 53:3:1060:U:H5''  | 1.97                     | 0.45              |
| 43:R:97:ARG:N     | 53:3:1307:U:H3'   | 2.30                     | 0.45              |
| 44:S:98:ALA:HB1   | 44:S:100:TRP:CE3  | 2.52                     | 0.45              |
| 47:V:11:VAL:HG21  | 47:V:20:ILE:HD11  | 1.98                     | 0.45              |
| 48:W:60:ARG:O     | 48:W:64:LEU:N     | 2.50                     | 0.45              |
| 49:X:52:ASN:HD21  | 49:X:55:GLN:CG    | 2.30                     | 0.45              |
| 50:Y:70:LYS:HE2   | 53:3:261:U:OP2    | 2.16                     | 0.45              |
| 53:3:337:G:H2'    | 53:3:338:A:H8     | 1.81                     | 0.45              |
| 53:3:398:U:O2'    | 53:3:399:G:H5'    | 2.16                     | 0.45              |
| 53:3:560:A:H5'    | 53:3:566:G:N2     | 2.30                     | 0.45              |
| 53:3:679:C:O2'    | 53:3:680:C:H5'    | 2.16                     | 0.45              |
| 53:3:1065:U:H5''  | 53:3:1190:G:H22   | 1.77                     | 0.45              |
| 53:3:1270:G:H2'   | 53:3:1271:A:C8    | 2.51                     | 0.45              |
| 54:1:694:U:H2'    | 54:1:695:G:H5''   | 1.97                     | 0.45              |
| 54:1:818:G:C2'    | 54:1:819:A:H5''   | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 54:1:1031:G:H2'  | 54:1:1032:A:C8   | 2.51                     | 0.45              |
| 54:1:1579:A:H2'  | 54:1:1580:A:C8   | 2.51                     | 0.45              |
| 54:1:2647:U:O2'  | 54:1:2648:G:H5'  | 2.16                     | 0.45              |
| 54:1:2727:A:O2'  | 54:1:2728:U:H5'  | 2.16                     | 0.45              |
| 1:b:229:HIS:ND1  | 1:b:230:PRO:HD2  | 2.31                     | 0.45              |
| 2:c:40:LEU:HD13  | 2:c:46:ARG:NH2   | 2.32                     | 0.45              |
| 3:d:189:THR:O    | 3:d:193:VAL:HG23 | 2.15                     | 0.45              |
| 4:e:84:ILE:HG12  | 54:1:2312:U:O4'  | 2.16                     | 0.45              |
| 4:e:110:ILE:CB   | 4:e:113:PHE:HB2  | 2.44                     | 0.45              |
| 4:e:149:ARG:H    | 4:e:149:ARG:CD   | 2.23                     | 0.45              |
| 7:h:37:LYS:HG2   | 7:h:41:LEU:HD12  | 1.98                     | 0.45              |
| 10:k:73:ASP:O    | 15:p:74:GLN:HG3  | 2.15                     | 0.45              |
| 10:k:105:ARG:C   | 10:k:107:LEU:H   | 2.24                     | 0.45              |
| 31:F:36:ARG:HD2  | 31:F:37:GLN:CG   | 2.42                     | 0.45              |
| 35:J:17:VAL:HA   | 35:J:34:ALA:HA   | 1.98                     | 0.45              |
| 41:P:14:GLN:HA   | 41:P:76:TYR:HA   | 1.98                     | 0.45              |
| 41:P:127:ARG:HB2 | 51:Z:34:ARG:NH2  | 2.31                     | 0.45              |
| 44:S:1:ALA:C     | 44:S:2:LYS:HD3   | 2.41                     | 0.45              |
| 49:X:11:ASP:HB3  | 49:X:14:LEU:HB3  | 1.98                     | 0.45              |
| 53:3:292:G:H2'   | 53:3:609:A:N1    | 2.32                     | 0.45              |
| 53:3:424:G:O2'   | 53:3:425:G:H5'   | 2.16                     | 0.45              |
| 53:3:1351:U:H3   | 53:3:1371:G:H1   | 1.63                     | 0.45              |
| 54:1:308:G:N2    | 54:1:329:G:H1'   | 2.31                     | 0.45              |
| 54:1:672:C:O2'   | 54:1:673:C:H5'   | 2.16                     | 0.45              |
| 54:1:940:G:H2'   | 54:1:941:A:H5''  | 1.98                     | 0.45              |
| 54:1:1213:A:H2'  | 54:1:1214:A:H8   | 1.81                     | 0.45              |
| 54:1:1311:G:H21  | 54:1:1603:A:H62  | 1.64                     | 0.45              |
| 54:1:1824:G:H2'  | 54:1:1825:U:C6   | 2.51                     | 0.45              |
| 54:1:2104:C:H42  | 54:1:2185:U:H3   | 1.64                     | 0.45              |
| 54:1:2292:U:H2'  | 54:1:2293:G:H8   | 1.82                     | 0.45              |
| 54:1:2584:U:H2'  | 54:1:2585:U:H2'  | 1.96                     | 0.45              |
| 54:1:2718:G:O2'  | 54:1:2847:U:H5'' | 2.16                     | 0.45              |
| 54:1:2828:G:O2'  | 54:1:2829:A:H5'  | 2.17                     | 0.45              |
| 2:c:161:MET:HE2  | 54:1:2050:C:H1'  | 1.99                     | 0.45              |
| 3:d:84:THR:OG1   | 54:1:586:A:H5'   | 2.16                     | 0.45              |
| 7:h:27:VAL:HG22  | 7:h:28:ALA:N     | 2.31                     | 0.45              |
| 7:h:56:ARG:HG3   | 7:h:82:ILE:O     | 2.16                     | 0.45              |
| 14:o:26:LEU:C    | 14:o:93:ASP:HB3  | 2.42                     | 0.45              |
| 15:p:2:ASN:O     | 15:p:6:GLN:HG2   | 2.16                     | 0.45              |
| 15:p:91:VAL:O    | 15:p:91:VAL:HG23 | 2.17                     | 0.45              |
| 16:q:111:LYS:CE  | 17:r:48:LYS:HZ1  | 2.26                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:D:44:VAL:HG13 | 29:D:44:VAL:O     | 2.17                     | 0.45              |
| 32:G:13:VAL:H    | 32:G:207:ARG:HH21 | 1.64                     | 0.45              |
| 34:I:54:LEU:HG   | 34:I:55:ARG:HH21  | 1.81                     | 0.45              |
| 34:I:67:LEU:HB3  | 53:3:546:A:OP2    | 2.16                     | 0.45              |
| 37:L:107:ALA:HB1 | 37:L:118:ARG:HB3  | 1.97                     | 0.45              |
| 37:L:129:ASN:CA  | 37:L:134:VAL:HG11 | 2.41                     | 0.45              |
| 40:O:87:LEU:O    | 40:O:88:MET:HE2   | 2.17                     | 0.45              |
| 41:P:68:ARG:HG3  | 41:P:68:ARG:HH11  | 1.81                     | 0.45              |
| 45:T:49:HIS:O    | 45:T:53:ARG:N     | 2.47                     | 0.45              |
| 46:U:21:VAL:HG21 | 46:U:60:TRP:CD1   | 2.51                     | 0.45              |
| 47:V:59:GLU:O    | 47:V:74:LEU:HD12  | 2.15                     | 0.45              |
| 49:X:9:PHE:O     | 49:X:38:THR:HG23  | 2.17                     | 0.45              |
| 50:Y:66:ILE:HG22 | 50:Y:67:HIS:N     | 2.30                     | 0.45              |
| 52:a:27:ILE:HG21 | 52:a:186:LYS:HB2  | 1.99                     | 0.45              |
| 53:3:212:G:H2'   | 53:3:213:G:C8     | 2.47                     | 0.45              |
| 53:3:252:U:O2    | 53:3:252:U:C2'    | 2.64                     | 0.45              |
| 53:3:321:A:O2'   | 53:3:322:C:H5'    | 2.17                     | 0.45              |
| 54:1:19:A:H5'    | 54:1:554:U:OP1    | 2.16                     | 0.45              |
| 54:1:44:A:H2'    | 54:1:45:G:O4'     | 2.16                     | 0.45              |
| 54:1:155:A:H2'   | 54:1:156:A:C8     | 2.51                     | 0.45              |
| 54:1:217:A:H2'   | 54:1:218:A:O4'    | 2.17                     | 0.45              |
| 54:1:468:G:H2'   | 54:1:469:G:O4'    | 2.17                     | 0.45              |
| 54:1:1386:C:H2'  | 54:1:1387:A:H8    | 1.81                     | 0.45              |
| 54:1:1508:A:H2'  | 54:1:1509:A:O4'   | 2.16                     | 0.45              |
| 54:1:2385:C:H2'  | 54:1:2386:A:C8    | 2.51                     | 0.45              |
| 59:8:364:VAL:HA  | 59:8:373:GLU:HA   | 1.98                     | 0.45              |
| 59:8:378:ARG:HA  | 59:8:378:ARG:HD3  | 1.72                     | 0.45              |
| 1:b:2:VAL:HG21   | 1:b:201:LEU:HD13  | 1.97                     | 0.45              |
| 1:b:16:VAL:CB    | 1:b:203:VAL:HG22  | 2.46                     | 0.45              |
| 7:h:46:ARG:NH1   | 7:h:46:ARG:HB2    | 2.32                     | 0.45              |
| 8:i:55:PRO:HG2   | 8:i:71:LYS:HB2    | 1.99                     | 0.45              |
| 9:j:71:ASP:O     | 9:j:73:VAL:HG23   | 2.15                     | 0.45              |
| 16:q:30:VAL:HG23 | 54:1:581:C:H5'    | 1.98                     | 0.45              |
| 18:s:16:LYS:O    | 18:s:19:LEU:HB2   | 2.17                     | 0.45              |
| 33:H:107:LYS:HD3 | 33:H:110:LEU:HD12 | 1.97                     | 0.45              |
| 35:J:17:VAL:HG22 | 35:J:18:ASN:N     | 2.30                     | 0.45              |
| 43:R:28:ARG:HH11 | 43:R:28:ARG:HG3   | 1.81                     | 0.45              |
| 43:R:106:ARG:CG  | 53:3:947:G:OP1    | 2.65                     | 0.45              |
| 44:S:19:TYR:HB3  | 44:S:20:PHE:H     | 1.54                     | 0.45              |
| 53:3:26:A:N6     | 53:3:558:G:H1'    | 2.31                     | 0.45              |
| 53:3:1121:U:H3   | 53:3:1152:A:N6    | 2.14                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:1150:A:H2'   | 53:3:1151:A:C8    | 2.51                     | 0.45              |
| 53:3:1197:A:H2'   | 53:3:1198:G:C5'   | 2.41                     | 0.45              |
| 54:1:146:A:H2'    | 54:1:147:C:H6     | 1.77                     | 0.45              |
| 54:1:343:C:C2'    | 54:1:344:A:H5'    | 2.47                     | 0.45              |
| 54:1:833:A:H2'    | 54:1:834:G:C8     | 2.51                     | 0.45              |
| 54:1:2391:G:C2'   | 54:1:2429:G:N2    | 2.79                     | 0.45              |
| 54:1:2443:C:H2'   | 54:1:2444:G:C8    | 2.52                     | 0.45              |
| 59:8:157:GLN:HA   | 59:8:160:THR:OG1  | 2.16                     | 0.45              |
| 59:8:397:LEU:N    | 59:8:397:LEU:HD12 | 2.31                     | 0.45              |
| 5:f:57:TYR:HB3    | 5:f:59:ASP:OD1    | 2.16                     | 0.45              |
| 5:f:88:LEU:HG     | 5:f:93:TYR:HB3    | 1.99                     | 0.45              |
| 9:j:88:THR:HG22   | 9:j:91:GLU:HG3    | 1.97                     | 0.45              |
| 10:k:35:VAL:HG11  | 10:k:106:GLU:HB3  | 1.98                     | 0.45              |
| 10:k:48:PRO:HG3   | 53:3:1422:G:H5'   | 1.99                     | 0.45              |
| 15:p:65:ASN:O     | 15:p:65:ASN:ND2   | 2.42                     | 0.45              |
| 16:q:105:PHE:O    | 16:q:109:VAL:HG23 | 2.16                     | 0.45              |
| 20:u:36:GLU:H     | 20:u:36:GLU:CD    | 2.24                     | 0.45              |
| 21:v:47:VAL:HA    | 21:v:50:MET:HG2   | 1.99                     | 0.45              |
| 24:y:49:ASP:O     | 24:y:53:VAL:HG23  | 2.16                     | 0.45              |
| 25:z:50:VAL:HB    | 25:z:53:MET:HG2   | 1.98                     | 0.45              |
| 32:G:69:VAL:HG12  | 32:G:70:GLY:N     | 2.32                     | 0.45              |
| 34:I:2:ARG:HD2    | 34:I:114:ARG:NH1  | 2.31                     | 0.45              |
| 34:I:158:LEU:HD23 | 34:I:158:LEU:C    | 2.42                     | 0.45              |
| 35:J:115:GLU:HG3  | 35:J:116:VAL:N    | 2.31                     | 0.45              |
| 35:J:164:LEU:HD12 | 35:J:164:LEU:C    | 2.42                     | 0.45              |
| 44:S:8:ARG:HE     | 53:3:1217:C:C5'   | 2.18                     | 0.45              |
| 44:S:57:SER:OG    | 53:3:1316:G:H4'   | 2.17                     | 0.45              |
| 49:X:14:LEU:C     | 49:X:14:LEU:HD23  | 2.42                     | 0.45              |
| 49:X:47:THR:HG22  | 49:X:60:PHE:CB    | 2.47                     | 0.45              |
| 52:a:27:ILE:O     | 52:a:31:LYS:HG2   | 2.16                     | 0.45              |
| 53:3:62:U:H2'     | 53:3:63:C:C6      | 2.51                     | 0.45              |
| 53:3:254:G:O2'    | 53:3:255:G:H5'    | 2.16                     | 0.45              |
| 53:3:360:G:O2'    | 53:3:361:G:H5'    | 2.17                     | 0.45              |
| 53:3:539:A:H2'    | 53:3:540:G:C8     | 2.52                     | 0.45              |
| 53:3:628:G:H2'    | 53:3:629:A:C8     | 2.51                     | 0.45              |
| 53:3:1497:G:O2'   | 53:3:1498:U:H5'   | 2.17                     | 0.45              |
| 54:1:150:U:H2'    | 54:1:151:C:H6     | 1.82                     | 0.45              |
| 54:1:2256:G:O2'   | 54:1:2257:U:H5'   | 2.17                     | 0.45              |
| 54:1:2331:G:H2'   | 54:1:2332:C:H6    | 1.80                     | 0.45              |
| 54:1:2443:C:H2'   | 54:1:2444:G:H8    | 1.80                     | 0.45              |
| 54:1:2593:U:H2'   | 54:1:2594:C:H6    | 1.82                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 54:1:2869:G:H2'  | 54:1:2870:C:O4'   | 2.17                     | 0.45              |
| 59:8:327:ASP:HB2 | 59:8:333:LEU:HD12 | 1.98                     | 0.45              |
| 59:8:539:ASP:HB3 | 59:8:578:LEU:O    | 2.16                     | 0.45              |
| 2:c:134:HIS:CE1  | 54:1:1675:C:C2    | 3.05                     | 0.45              |
| 4:e:21:TYR:HB3   | 4:e:26:GLN:HB3    | 1.99                     | 0.45              |
| 4:e:78:ILE:HG13  | 4:e:78:ILE:O      | 2.17                     | 0.45              |
| 6:g:4:ILE:HG22   | 6:g:37:VAL:O      | 2.16                     | 0.45              |
| 9:j:2:LYS:HE2    | 9:j:2:LYS:HA      | 1.97                     | 0.45              |
| 30:E:13:PHE:O    | 30:E:14:LYS:HD2   | 2.17                     | 0.45              |
| 37:L:76:SER:OG   | 37:L:83:THR:HB    | 2.17                     | 0.45              |
| 41:P:111:ASP:OD2 | 41:P:113:THR:HG23 | 2.16                     | 0.45              |
| 44:S:79:SER:OG   | 44:S:82:LYS:HG2   | 2.17                     | 0.45              |
| 44:S:80:ARG:HG3  | 44:S:80:ARG:NH1   | 2.31                     | 0.45              |
| 47:V:64:ARG:HD2  | 53:3:264:C:H4'    | 1.99                     | 0.45              |
| 51:Z:49:ALA:HA   | 53:3:723:U:O4     | 2.17                     | 0.45              |
| 53:3:45:G:H2'    | 53:3:46:G:C8      | 2.52                     | 0.45              |
| 53:3:378:G:H2'   | 53:3:379:C:C6     | 2.51                     | 0.45              |
| 53:3:502:A:O2'   | 53:3:503:C:H5'    | 2.17                     | 0.45              |
| 53:3:593:U:H2'   | 53:3:594:U:C6     | 2.52                     | 0.45              |
| 53:3:1058:G:H2'  | 53:3:1059:C:O4'   | 2.15                     | 0.45              |
| 53:3:1300:G:O2'  | 53:3:1303:C:N4    | 2.49                     | 0.45              |
| 53:3:1347:G:N2   | 53:3:1373:G:H2'   | 2.31                     | 0.45              |
| 54:1:593:U:H2'   | 54:1:594:U:H6     | 1.76                     | 0.45              |
| 54:1:672:C:H2'   | 54:1:673:C:C6     | 2.52                     | 0.45              |
| 54:1:1600:C:O2'  | 54:1:1601:G:H5'   | 2.16                     | 0.45              |
| 54:1:2417:C:O2'  | 54:1:2418:A:H5'   | 2.16                     | 0.45              |
| 57:6:37:A:C6     | 57:6:38:A:N7      | 2.85                     | 0.45              |
| 59:8:159:LYS:NZ  | 59:8:166:PRO:HD2  | 2.32                     | 0.45              |
| 59:8:252:LEU:O   | 59:8:255:ARG:N    | 2.49                     | 0.45              |
| 59:8:544:VAL:O   | 59:8:544:VAL:HG12 | 2.16                     | 0.45              |
| 1:b:66:PHE:HB3   | 1:b:150:GLY:O     | 2.17                     | 0.45              |
| 3:d:19:PHE:CE2   | 3:d:188:MET:HE1   | 2.52                     | 0.45              |
| 4:e:166:ARG:HH11 | 4:e:166:ARG:HB3   | 1.80                     | 0.45              |
| 4:e:169:LEU:HD22 | 4:e:174:PHE:CE1   | 2.52                     | 0.45              |
| 4:e:169:LEU:HD13 | 4:e:174:PHE:CE1   | 2.52                     | 0.45              |
| 5:f:46:ASP:OD2   | 5:f:48:THR:HG23   | 2.17                     | 0.45              |
| 7:h:58:THR:CB    | 7:h:82:ILE:HB     | 2.47                     | 0.45              |
| 14:o:26:LEU:O    | 14:o:93:ASP:HB3   | 2.16                     | 0.45              |
| 20:u:94:PHE:CZ   | 20:u:96:LYS:HD3   | 2.52                     | 0.45              |
| 31:F:36:ARG:CG   | 31:F:37:GLN:H     | 2.30                     | 0.45              |
| 32:G:26:MET:HE2  | 32:G:190:SER:C    | 2.41                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:I:183:ARG:HG2 | 34:I:183:ARG:NH1 | 2.31                     | 0.45              |
| 39:N:87:MET:HG2  | 39:N:88:GLU:N    | 2.31                     | 0.45              |
| 40:O:36:VAL:HG22 | 53:3:1123:U:H5'  | 1.98                     | 0.45              |
| 40:O:44:THR:HB   | 40:O:69:THR:O    | 2.17                     | 0.45              |
| 42:Q:57:THR:OG1  | 53:3:362:G:H5''  | 2.17                     | 0.45              |
| 44:S:51:PRO:HG2  | 44:S:54:SER:OG   | 2.16                     | 0.45              |
| 48:W:25:ILE:HD13 | 48:W:28:LEU:HD12 | 1.99                     | 0.45              |
| 50:Y:79:THR:HA   | 50:Y:82:ILE:HG12 | 1.98                     | 0.45              |
| 53:3:15:G:H22    | 53:3:1080:A:C4'  | 2.29                     | 0.45              |
| 53:3:20:U:O2'    | 53:3:21:G:H5'    | 2.17                     | 0.45              |
| 53:3:441:A:H5'   | 53:3:442:G:OP2   | 2.17                     | 0.45              |
| 53:3:577:G:H2'   | 53:3:578:C:C6    | 2.51                     | 0.45              |
| 53:3:943:U:H2'   | 53:3:944:G:C8    | 2.52                     | 0.45              |
| 53:3:946:A:O4'   | 53:3:1334:G:H4'  | 2.17                     | 0.45              |
| 53:3:1104:G:O2'  | 53:3:1105:A:H5'  | 2.16                     | 0.45              |
| 53:3:1256:A:H1'  | 53:3:1258:G:C8   | 2.52                     | 0.45              |
| 54:1:391:A:H1'   | 54:1:411:G:O4'   | 2.17                     | 0.45              |
| 54:1:1139:G:H2'  | 54:1:1140:C:C6   | 2.50                     | 0.45              |
| 54:1:1177:G:H2'  | 54:1:1178:C:O4'  | 2.17                     | 0.45              |
| 54:1:2650:U:H2'  | 54:1:2651:C:C6   | 2.52                     | 0.45              |
| 1:b:156:SER:HB3  | 1:b:159:THR:HG21 | 1.99                     | 0.45              |
| 1:b:241:LYS:O    | 54:1:1902:C:H4'  | 2.16                     | 0.45              |
| 4:e:70:ARG:HH22  | 4:e:71:LYS:HD3   | 1.81                     | 0.45              |
| 4:e:141:ASP:H    | 4:e:144:LYS:HG2  | 1.82                     | 0.45              |
| 4:e:141:ASP:C    | 4:e:143:ASP:H    | 2.25                     | 0.45              |
| 5:f:4:ALA:HB2    | 5:f:65:GLY:HA2   | 1.99                     | 0.45              |
| 5:f:8:VAL:HG22   | 5:f:68:ARG:NE    | 2.32                     | 0.45              |
| 7:h:57:ASN:O     | 7:h:62:ARG:HB3   | 2.17                     | 0.45              |
| 11:l:78:ARG:CZ   | 11:l:113:ALA:HB1 | 2.47                     | 0.45              |
| 12:m:50:ARG:HG2  | 12:m:50:ARG:HH21 | 1.80                     | 0.45              |
| 13:n:78:LYS:HG3  | 13:n:82:GLU:OE2  | 2.17                     | 0.45              |
| 15:p:19:PHE:N    | 15:p:19:PHE:CD1  | 2.84                     | 0.45              |
| 25:z:40:THR:O    | 25:z:44:ARG:HG2  | 2.17                     | 0.45              |
| 34:I:171:GLU:HB2 | 34:I:182:LYS:HG3 | 1.98                     | 0.45              |
| 34:I:205:LYS:HB3 | 53:3:8:A:N1      | 2.32                     | 0.45              |
| 35:J:96:GLN:HE21 | 35:J:123:LEU:CD1 | 2.29                     | 0.45              |
| 38:M:26:MET:O    | 38:M:58:LEU:N    | 2.46                     | 0.45              |
| 41:P:55:ARG:HG2  | 41:P:55:ARG:HH11 | 1.82                     | 0.45              |
| 42:Q:35:ARG:HA   | 42:Q:35:ARG:HE   | 1.81                     | 0.45              |
| 44:S:12:ARG:NH1  | 44:S:12:ARG:HB2  | 2.31                     | 0.45              |
| 53:3:878:A:H2'   | 53:3:879:C:H6    | 1.78                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:3:1097:C:O2'  | 53:3:1098:C:H5'   | 2.17                     | 0.45              |
| 53:3:1277:C:H5'' | 53:3:1281:C:H42   | 1.82                     | 0.45              |
| 53:3:1432:G:H1'  | 53:3:1468:A:N6    | 2.32                     | 0.45              |
| 54:1:594:U:H2'   | 54:1:595:C:H6     | 1.81                     | 0.45              |
| 54:1:745:G:O2'   | 54:1:748:G:H1'    | 2.16                     | 0.45              |
| 54:1:1318:U:H2'  | 54:1:1319:C:C6    | 2.51                     | 0.45              |
| 54:1:1469:A:H2'  | 54:1:1470:A:C8    | 2.52                     | 0.45              |
| 59:8:10:TYR:O    | 59:8:11:ARG:HG3   | 2.17                     | 0.45              |
| 59:8:253:ARG:HA  | 59:8:256:VAL:HG22 | 1.99                     | 0.45              |
| 1:b:148:GLY:O    | 54:1:2205:A:H5'   | 2.17                     | 0.45              |
| 2:c:105:LYS:O    | 2:c:177:VAL:HG12  | 2.16                     | 0.45              |
| 13:n:65:LEU:CG   | 13:n:69:ARG:HH22  | 2.29                     | 0.45              |
| 15:p:93:LYS:HE3  | 54:1:1754:A:C8    | 2.52                     | 0.45              |
| 17:r:6:GLN:HG2   | 17:r:11:GLN:HE21  | 1.82                     | 0.45              |
| 17:r:75:VAL:HG22 | 17:r:86:GLN:NE2   | 2.32                     | 0.45              |
| 24:y:46:VAL:O    | 24:y:50:VAL:HG23  | 2.16                     | 0.45              |
| 38:M:6:ILE:HD13  | 38:M:32:LYS:CE    | 2.45                     | 0.45              |
| 39:N:83:THR:HG21 | 39:N:103:VAL:HG12 | 1.98                     | 0.45              |
| 40:O:65:TYR:CD2  | 44:S:95:LEU:HD11  | 2.52                     | 0.45              |
| 43:R:56:ARG:O    | 43:R:59:VAL:HG22  | 2.17                     | 0.45              |
| 44:S:27:LYS:O    | 44:S:31:SER:HB3   | 2.17                     | 0.45              |
| 51:Z:32:ARG:CD   | 51:Z:33:ARG:HG2   | 2.47                     | 0.45              |
| 53:3:16:A:H2'    | 53:3:17:U:H5'     | 1.97                     | 0.45              |
| 53:3:243:A:C2    | 53:3:245:U:H2'    | 2.52                     | 0.45              |
| 53:3:951:G:C2'   | 53:3:952:U:H5'    | 2.47                     | 0.45              |
| 53:3:1109:C:O5'  | 53:3:1109:C:H6    | 1.99                     | 0.45              |
| 54:1:144:A:H2'   | 54:1:145:C:C6     | 2.52                     | 0.45              |
| 54:1:705:A:H62   | 54:1:726:G:H1'    | 1.82                     | 0.45              |
| 54:1:1073:A:H2'  | 54:1:1074:G:O4'   | 2.17                     | 0.45              |
| 54:1:1447:C:H2'  | 54:1:1448:G:H8    | 1.82                     | 0.45              |
| 54:1:2174:C:O2'  | 54:1:2175:C:H5'   | 2.17                     | 0.45              |
| 54:1:2533:U:H2'  | 54:1:2534:A:O4'   | 2.17                     | 0.45              |
| 54:1:2579:C:O2'  | 54:1:2580:U:H5'   | 2.17                     | 0.45              |
| 54:1:2758:A:H2'  | 54:1:2759:G:O4'   | 2.16                     | 0.45              |
| 54:1:2837:A:H2'  | 54:1:2838:G:H8    | 1.82                     | 0.45              |
| 55:2:56:G:H4'    | 55:2:57:A:H8      | 1.81                     | 0.45              |
| 57:6:38:A:H3'    | 57:6:39:C:C5      | 2.51                     | 0.45              |
| 3:d:17:THR:O     | 3:d:21:ARG:HB2    | 2.17                     | 0.45              |
| 3:d:102:ARG:O    | 3:d:106:LYS:HG3   | 2.16                     | 0.45              |
| 3:d:147:LEU:HD12 | 3:d:168:ASP:HB3   | 1.98                     | 0.45              |
| 4:e:39:VAL:HG13  | 4:e:40:GLY:N      | 2.28                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:m:2:LEU:HB3    | 12:m:68:PHE:CE1   | 2.52                     | 0.45              |
| 15:p:102:ARG:HH21 | 54:1:1754:A:H4'   | 1.82                     | 0.45              |
| 16:q:91:ARG:HD2   | 16:q:91:ARG:H     | 1.81                     | 0.45              |
| 18:s:89:ALA:O     | 18:s:92:ARG:NH1   | 2.50                     | 0.45              |
| 25:z:9:THR:HG23   | 25:z:10:ARG:HG2   | 1.99                     | 0.45              |
| 25:z:56:VAL:HG22  | 25:z:58:GLU:HG3   | 1.98                     | 0.45              |
| 30:E:32:LEU:HD12  | 54:1:2420:C:OP2   | 2.17                     | 0.45              |
| 32:G:99:MET:HG3   | 32:G:100:LEU:CD1  | 2.46                     | 0.45              |
| 32:G:221:ARG:HB2  | 32:G:221:ARG:NH1  | 2.31                     | 0.45              |
| 35:J:40:ASP:OD2   | 35:J:44:ARG:HB2   | 2.17                     | 0.45              |
| 37:L:110:ARG:O    | 37:L:112:ASP:N    | 2.49                     | 0.45              |
| 42:Q:37:TYR:CE1   | 42:Q:51:VAL:HG13  | 2.52                     | 0.45              |
| 42:Q:51:VAL:HG22  | 42:Q:52:CYS:N     | 2.32                     | 0.45              |
| 43:R:69:ARG:NH1   | 43:R:69:ARG:CB    | 2.80                     | 0.45              |
| 43:R:106:ARG:O    | 43:R:110:GLY:N    | 2.50                     | 0.45              |
| 44:S:92:ILE:HD12  | 44:S:92:ILE:H     | 1.81                     | 0.45              |
| 53:3:16:A:N1      | 53:3:1080:A:C5    | 2.85                     | 0.45              |
| 53:3:945:G:N1     | 53:3:946:A:C8     | 2.84                     | 0.45              |
| 53:3:1375:A:H2'   | 53:3:1376:U:C6    | 2.52                     | 0.45              |
| 53:3:1413:A:H2    | 53:3:1487:G:H22   | 1.65                     | 0.45              |
| 54:1:52:A:H2'     | 54:1:53:A:H8      | 1.81                     | 0.45              |
| 54:1:381:G:O2'    | 54:1:382:A:H5'    | 2.16                     | 0.45              |
| 54:1:644:A:H2'    | 54:1:645:C:O4'    | 2.17                     | 0.45              |
| 54:1:2065:C:H1'   | 54:1:2449:U:H3    | 1.82                     | 0.45              |
| 54:1:2149:U:H2'   | 54:1:2150:C:O4'   | 2.17                     | 0.45              |
| 56:5:17:U:OP1     | 56:5:61:C:H5'     | 2.16                     | 0.45              |
| 59:8:109:ALA:HB3  | 59:8:137:ARG:CB   | 2.47                     | 0.45              |
| 59:8:152:LEU:HD23 | 59:8:152:LEU:H    | 1.82                     | 0.45              |
| 59:8:194:ASN:CG   | 59:8:195:ASP:H    | 2.24                     | 0.45              |
| 59:8:334:THR:HG21 | 59:8:388:LEU:HD13 | 1.99                     | 0.45              |
| 8:i:19:PRO:HB2    | 8:i:23:VAL:HG23   | 1.99                     | 0.44              |
| 9:j:57:LEU:O      | 9:j:58:ASN:HB2    | 2.16                     | 0.44              |
| 10:k:31:ARG:HG2   | 10:k:31:ARG:HH11  | 1.82                     | 0.44              |
| 11:l:135:ILE:HB   | 11:l:142:ILE:HD11 | 2.00                     | 0.44              |
| 12:m:135:VAL:O    | 12:m:136:MET:HG2  | 2.18                     | 0.44              |
| 19:t:34:VAL:HG22  | 19:t:81:LYS:O     | 2.17                     | 0.44              |
| 27:B:27:LEU:HD23  | 27:B:36:LYS:HE2   | 1.98                     | 0.44              |
| 31:F:30:GLU:OE2   | 31:F:32:LYS:HG3   | 2.18                     | 0.44              |
| 32:G:15:PHE:N     | 32:G:202:ASN:ND2  | 2.65                     | 0.44              |
| 35:J:24:VAL:C     | 35:J:26:GLY:H     | 2.24                     | 0.44              |
| 36:K:6:ILE:HD11   | 36:K:78:PHE:CE2   | 2.52                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:K:8:PHE:CD1    | 36:K:62:MET:HE1   | 2.53                     | 0.44              |
| 40:O:85:ASP:OD2   | 40:O:89:ARG:NH2   | 2.50                     | 0.44              |
| 46:U:70:ARG:HD3   | 53:3:375:U:OP1    | 2.17                     | 0.44              |
| 48:W:33:THR:HG23  | 48:W:36:GLY:H     | 1.81                     | 0.44              |
| 52:a:27:ILE:HD12  | 52:a:182:ALA:C    | 2.43                     | 0.44              |
| 53:3:915:A:H2'    | 53:3:916:U:H5'    | 1.98                     | 0.44              |
| 53:3:998:C:O2'    | 53:3:999:C:H5'    | 2.17                     | 0.44              |
| 54:1:161:A:H3'    | 54:1:162:U:H5''   | 1.98                     | 0.44              |
| 54:1:433:C:O2'    | 54:1:434:U:H5'    | 2.16                     | 0.44              |
| 54:1:691:C:H2'    | 54:1:692:C:H6     | 1.81                     | 0.44              |
| 54:1:1664:A:H61   | 54:1:1996:C:N4    | 2.08                     | 0.44              |
| 54:1:2658:C:H2'   | 54:1:2659:G:O4'   | 2.16                     | 0.44              |
| 56:5:3:G:C4       | 56:5:4:C:C5       | 3.05                     | 0.44              |
| 56:5:15:G:H22     | 56:5:48:C:H42     | 1.65                     | 0.44              |
| 59:8:56:GLU:HG3   | 59:8:61:ILE:C     | 2.41                     | 0.44              |
| 59:8:618:LYS:HB2  | 59:8:685:LEU:HD12 | 1.99                     | 0.44              |
| 2:c:149:ASN:HD22  | 54:1:2572:A:H2'   | 1.82                     | 0.44              |
| 5:f:66:THR:OG1    | 54:1:2748:A:H1'   | 2.16                     | 0.44              |
| 13:n:69:ARG:C     | 13:n:70:THR:HG23  | 2.42                     | 0.44              |
| 17:r:75:VAL:HG22  | 17:r:86:GLN:HE22  | 1.82                     | 0.44              |
| 27:B:51:ARG:HG2   | 27:B:52:LYS:N     | 2.32                     | 0.44              |
| 35:J:33:THR:HG22  | 35:J:51:LYS:CB    | 2.46                     | 0.44              |
| 38:M:10:LEU:HD11  | 38:M:76:ARG:HB2   | 1.99                     | 0.44              |
| 39:N:44:ARG:H     | 39:N:44:ARG:HD3   | 1.82                     | 0.44              |
| 39:N:112:ARG:HD3  | 44:S:100:TRP:CD1  | 2.52                     | 0.44              |
| 39:N:118:ARG:HH11 | 39:N:118:ARG:HG3  | 1.82                     | 0.44              |
| 40:O:59:LYS:HE3   | 40:O:62:ARG:NH2   | 2.32                     | 0.44              |
| 43:R:19:THR:HA    | 43:R:24:VAL:CG2   | 2.47                     | 0.44              |
| 44:S:60:ARG:O     | 44:S:61:ASN:HB2   | 2.17                     | 0.44              |
| 46:U:75:ILE:HG22  | 46:U:80:LYS:HE3   | 1.99                     | 0.44              |
| 47:V:12:VAL:HG21  | 47:V:42:LYS:NZ    | 2.31                     | 0.44              |
| 47:V:57:VAL:HB    | 47:V:78:VAL:HG23  | 1.99                     | 0.44              |
| 52:a:189:LEU:HD11 | 52:a:212:VAL:CG1  | 2.47                     | 0.44              |
| 52:a:193:LEU:O    | 52:a:197:LYS:HG3  | 2.17                     | 0.44              |
| 53:3:665:A:O4'    | 53:3:733:G:H1'    | 2.16                     | 0.44              |
| 53:3:1166:G:H21   | 53:3:1168:U:P     | 2.40                     | 0.44              |
| 53:3:1172:C:H2'   | 53:3:1173:U:H6    | 1.81                     | 0.44              |
| 53:3:1349:A:C1'   | 53:3:1374:A:N6    | 2.80                     | 0.44              |
| 54:1:5:A:H2'      | 54:1:6:A:C8       | 2.53                     | 0.44              |
| 54:1:52:A:H2'     | 54:1:53:A:C8      | 2.52                     | 0.44              |
| 54:1:784:G:OP1    | 54:1:2588:G:H5''  | 2.16                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:1106:G:H5'   | 54:1:1106:G:H8    | 1.81                     | 0.44              |
| 54:1:1316:U:H2'   | 54:1:1317:G:H8    | 1.82                     | 0.44              |
| 54:1:1439:A:H2'   | 54:1:1440:U:H5'   | 1.99                     | 0.44              |
| 54:1:2052:A:O2'   | 54:1:2053:G:H5'   | 2.18                     | 0.44              |
| 54:1:2412:A:H2'   | 54:1:2413:G:O4'   | 2.17                     | 0.44              |
| 54:1:2639:A:H2'   | 54:1:2640:G:O4'   | 2.18                     | 0.44              |
| 3:d:73:ILE:O      | 3:d:73:ILE:HG12   | 2.17                     | 0.44              |
| 12:m:80:VAL:HG12  | 12:m:81:ARG:O     | 2.18                     | 0.44              |
| 21:v:12:GLN:OE1   | 21:v:12:GLN:N     | 2.51                     | 0.44              |
| 26:A:58:ASP:O     | 26:A:62:LYS:N     | 2.50                     | 0.44              |
| 33:H:142:ARG:HH11 | 33:H:142:ARG:HB2  | 1.82                     | 0.44              |
| 34:I:120:LYS:HB3  | 34:I:128:VAL:HG21 | 1.99                     | 0.44              |
| 35:J:44:ARG:HH21  | 35:J:70:MET:HG3   | 1.81                     | 0.44              |
| 35:J:114:LEU:O    | 35:J:119:VAL:HG22 | 2.18                     | 0.44              |
| 36:K:6:ILE:HG13   | 36:K:88:MET:O     | 2.17                     | 0.44              |
| 36:K:29:ILE:HD13  | 36:K:64:VAL:HG21  | 1.99                     | 0.44              |
| 40:O:40:ILE:N     | 53:3:1123:U:C2    | 2.86                     | 0.44              |
| 44:S:10:VAL:HA    | 44:S:13:VAL:HG23  | 1.99                     | 0.44              |
| 44:S:12:ARG:HG2   | 44:S:59:GLN:HG2   | 2.00                     | 0.44              |
| 51:Z:6:ARG:HG2    | 51:Z:8:ASN:HA     | 2.00                     | 0.44              |
| 51:Z:52:VAL:HA    | 51:Z:55:HIS:HB2   | 2.00                     | 0.44              |
| 51:Z:65:ARG:HH11  | 51:Z:65:ARG:HG2   | 1.83                     | 0.44              |
| 53:3:197:A:N3     | 53:3:198:G:H1'    | 2.33                     | 0.44              |
| 53:3:451:A:H4'    | 53:3:452:A:C5'    | 2.48                     | 0.44              |
| 53:3:925:G:C2     | 53:3:927:G:N7     | 2.85                     | 0.44              |
| 53:3:1171:A:H2'   | 53:3:1172:C:O4'   | 2.17                     | 0.44              |
| 53:3:1242:G:H4'   | 53:3:1304:G:OP1   | 2.18                     | 0.44              |
| 54:1:23:G:H2'     | 54:1:24:G:C8      | 2.51                     | 0.44              |
| 54:1:570:G:H2'    | 54:1:2030:A:N7    | 2.33                     | 0.44              |
| 54:1:691:C:H2'    | 54:1:692:C:C6     | 2.53                     | 0.44              |
| 54:1:832:U:H2'    | 54:1:833:A:C8     | 2.53                     | 0.44              |
| 54:1:1062:G:N3    | 54:1:1062:G:H2'   | 2.32                     | 0.44              |
| 54:1:1219:U:H2'   | 54:1:1220:G:H8    | 1.81                     | 0.44              |
| 54:1:1344:U:H3'   | 54:1:1345:C:H5'   | 1.99                     | 0.44              |
| 54:1:2519:U:H5'   | 54:1:2567:G:N2    | 2.31                     | 0.44              |
| 54:1:2715:C:H3'   | 54:1:2716:C:H5''  | 1.99                     | 0.44              |
| 55:2:97:C:H2'     | 55:2:98:G:H5'     | 1.98                     | 0.44              |
| 59:8:236:LYS:O    | 59:8:241:GLU:N    | 2.43                     | 0.44              |
| 1:b:71:ASP:O      | 1:b:73:ILE:HG13   | 2.18                     | 0.44              |
| 6:g:94:ILE:CD1    | 6:g:122:LEU:HD13  | 2.47                     | 0.44              |
| 7:h:26:VAL:HG12   | 7:h:82:ILE:CG2    | 2.47                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:k:107:LEU:O   | 10:k:109:SER:N   | 2.44                     | 0.44              |
| 21:v:28:ALA:HB3  | 21:v:40:ILE:HB   | 1.99                     | 0.44              |
| 32:G:57:ASN:HA   | 32:G:60:ALA:HB3  | 1.99                     | 0.44              |
| 34:I:25:ARG:NH1  | 34:I:30:LYS:NZ   | 2.64                     | 0.44              |
| 34:I:38:GLY:HA3  | 53:3:542:G:H5'   | 1.98                     | 0.44              |
| 35:J:24:VAL:HG12 | 35:J:29:ILE:CG1  | 2.48                     | 0.44              |
| 35:J:132:PRO:HA  | 35:J:135:VAL:HB  | 2.00                     | 0.44              |
| 36:K:74:LEU:HG   | 36:K:78:PHE:CE1  | 2.52                     | 0.44              |
| 41:P:24:ALA:N    | 41:P:86:LYS:O    | 2.45                     | 0.44              |
| 43:R:98:GLY:H    | 53:3:1308:U:H6   | 1.65                     | 0.44              |
| 44:S:44:VAL:HA   | 44:S:47:LEU:HB2  | 1.98                     | 0.44              |
| 47:V:21:VAL:HA   | 47:V:43:LEU:O    | 2.17                     | 0.44              |
| 48:W:38:ILE:HG13 | 53:3:719:C:O2    | 2.18                     | 0.44              |
| 48:W:54:LEU:HD12 | 48:W:55:ALA:N    | 2.33                     | 0.44              |
| 49:X:4:LEU:HD21  | 49:X:9:PHE:HB2   | 2.00                     | 0.44              |
| 51:Z:44:ARG:C    | 51:Z:44:ARG:CD   | 2.90                     | 0.44              |
| 53:3:613:C:H2'   | 53:3:614:C:C6    | 2.52                     | 0.44              |
| 53:3:635:A:H2'   | 53:3:636:U:C6    | 2.53                     | 0.44              |
| 54:1:167:A:H2'   | 54:1:168:G:O4'   | 2.17                     | 0.44              |
| 54:1:634:C:H2'   | 54:1:635:C:H6    | 1.83                     | 0.44              |
| 54:1:677:A:N6    | 54:1:802:A:N7    | 2.65                     | 0.44              |
| 54:1:677:A:H2'   | 54:1:678:C:H6    | 1.82                     | 0.44              |
| 54:1:1219:U:H2'  | 54:1:1220:G:C8   | 2.52                     | 0.44              |
| 54:1:2391:G:H2'  | 54:1:2429:G:N2   | 2.32                     | 0.44              |
| 59:8:77:LYS:C    | 59:8:79:TYR:H    | 2.25                     | 0.44              |
| 59:8:496:GLN:HG2 | 59:8:608:ALA:HA  | 1.99                     | 0.44              |
| 4:e:169:LEU:HB3  | 4:e:174:PHE:CD1  | 2.52                     | 0.44              |
| 15:p:25:VAL:HG12 | 15:p:26:GLU:N    | 2.33                     | 0.44              |
| 15:p:77:SER:OG   | 15:p:79:VAL:HG12 | 2.17                     | 0.44              |
| 16:q:91:ARG:HD3  | 54:1:997:G:OP1   | 2.18                     | 0.44              |
| 20:u:13:LEU:HD11 | 20:u:70:ALA:HB2  | 1.99                     | 0.44              |
| 21:v:86:LEU:HD23 | 21:v:89:ILE:HD11 | 1.99                     | 0.44              |
| 25:z:10:ARG:NH2  | 25:z:10:ARG:HG3  | 2.32                     | 0.44              |
| 28:C:5:ARG:HH11  | 28:C:25:ASN:HB2  | 1.78                     | 0.44              |
| 32:G:69:VAL:N    | 32:G:161:PHE:O   | 2.47                     | 0.44              |
| 47:V:13:SER:H    | 47:V:21:VAL:HG13 | 1.83                     | 0.44              |
| 48:W:55:ALA:O    | 48:W:59:LYS:HG3  | 2.18                     | 0.44              |
| 48:W:61:ALA:HB1  | 48:W:67:LEU:HG   | 1.99                     | 0.44              |
| 53:3:270:A:H2'   | 53:3:271:C:H6    | 1.80                     | 0.44              |
| 53:3:677:U:H2'   | 53:3:678:U:C6    | 2.53                     | 0.44              |
| 53:3:701:U:H4'   | 53:3:703:G:H1'   | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:791:G:C6     | 53:3:792:A:N7     | 2.86                     | 0.44              |
| 53:3:797:C:O2'    | 53:3:798:U:H5'    | 2.17                     | 0.44              |
| 53:3:1054:C:H4'   | 53:3:1056:U:OP2   | 2.17                     | 0.44              |
| 53:3:1064:G:O2'   | 53:3:1190:G:N2    | 2.50                     | 0.44              |
| 53:3:1513:A:N1    | 53:3:1523:G:C6    | 2.85                     | 0.44              |
| 54:1:178:G:O2'    | 54:1:179:C:H5'    | 2.17                     | 0.44              |
| 54:1:391:A:H2'    | 54:1:391:A:N3     | 2.33                     | 0.44              |
| 54:1:1372:U:O2'   | 54:1:1373:A:H5'   | 2.18                     | 0.44              |
| 54:1:1635:A:H2'   | 54:1:1636:U:O4'   | 2.18                     | 0.44              |
| 54:1:2024:G:H2'   | 54:1:2025:C:H6    | 1.82                     | 0.44              |
| 54:1:2556:C:H2'   | 54:1:2557:G:O4'   | 2.18                     | 0.44              |
| 54:1:2742:G:O2'   | 54:1:2743:U:H5'   | 2.18                     | 0.44              |
| 54:1:2743:U:H2'   | 54:1:2744:G:O4'   | 2.18                     | 0.44              |
| 54:1:2744:G:O2'   | 54:1:2745:C:H5'   | 2.18                     | 0.44              |
| 54:1:2757:A:H2'   | 54:1:2757:A:N3    | 2.33                     | 0.44              |
| 59:8:192:ASN:O    | 59:8:203:GLU:HB2  | 2.17                     | 0.44              |
| 59:8:244:THR:HB   | 59:8:247:GLU:CB   | 2.47                     | 0.44              |
| 59:8:544:VAL:HG12 | 59:8:582:SER:HA   | 1.99                     | 0.44              |
| 1:b:229:HIS:CE1   | 1:b:230:PRO:HD2   | 2.52                     | 0.44              |
| 11:l:71:ALA:O     | 11:l:74:THR:HG22  | 2.18                     | 0.44              |
| 11:l:76:GLU:C     | 11:l:77:ILE:HD12  | 2.43                     | 0.44              |
| 11:l:103:ILE:O    | 11:l:103:ILE:HG22 | 2.17                     | 0.44              |
| 14:o:99:TYR:CE1   | 14:o:104:GLN:HA   | 2.52                     | 0.44              |
| 15:p:95:LYS:HG3   | 54:1:2718:G:O3'   | 2.17                     | 0.44              |
| 19:t:29:THR:HG21  | 19:t:86:THR:HG22  | 1.98                     | 0.44              |
| 36:K:8:PHE:HD1    | 36:K:62:MET:HE1   | 1.82                     | 0.44              |
| 36:K:18:VAL:HG13  | 36:K:19:PRO:CD    | 2.48                     | 0.44              |
| 37:L:22:LEU:HD12  | 37:L:25:PHE:CB    | 2.36                     | 0.44              |
| 38:M:45:ILE:HG22  | 38:M:46:GLU:O     | 2.18                     | 0.44              |
| 39:N:30:ASN:O     | 39:N:32:ARG:HG2   | 2.17                     | 0.44              |
| 47:V:7:LEU:HD12   | 47:V:7:LEU:N      | 2.33                     | 0.44              |
| 49:X:76:THR:HG21  | 53:3:1321:U:H1'   | 1.99                     | 0.44              |
| 51:Z:11:PHE:C     | 51:Z:13:VAL:N     | 2.75                     | 0.44              |
| 51:Z:25:ALA:O     | 51:Z:29:ALA:N     | 2.36                     | 0.44              |
| 53:3:382:A:O2'    | 53:3:383:A:H5'    | 2.18                     | 0.44              |
| 53:3:487:A:H2'    | 53:3:488:C:O4'    | 2.18                     | 0.44              |
| 53:3:686:U:O2     | 53:3:704:A:N7     | 2.50                     | 0.44              |
| 53:3:1017:U:H2'   | 53:3:1018:G:C8    | 2.52                     | 0.44              |
| 53:3:1463:U:H2'   | 53:3:1464:U:C6    | 2.52                     | 0.44              |
| 53:3:1540:U:O2    | 53:3:1540:U:H3'   | 2.17                     | 0.44              |
| 54:1:69:C:H2'     | 54:1:70:G:H8      | 1.83                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:539:G:H2'    | 54:1:540:C:C6     | 2.52                     | 0.44              |
| 54:1:634:C:O5'    | 54:1:634:C:H6     | 2.00                     | 0.44              |
| 54:1:759:G:H2'    | 54:1:760:G:C8     | 2.53                     | 0.44              |
| 54:1:1098:A:H2'   | 54:1:1099:G:O4'   | 2.17                     | 0.44              |
| 54:1:1190:G:H2'   | 54:1:1191:G:C8    | 2.52                     | 0.44              |
| 54:1:1826:G:H2'   | 54:1:1827:U:C6    | 2.52                     | 0.44              |
| 54:1:1858:A:H1'   | 54:1:1885:A:C2    | 2.52                     | 0.44              |
| 54:1:2194:U:H2'   | 54:1:2195:U:C6    | 2.52                     | 0.44              |
| 59:8:142:ASN:CG   | 59:8:143:LYS:N    | 2.76                     | 0.44              |
| 59:8:603:GLU:O    | 59:8:607:LYS:N    | 2.49                     | 0.44              |
| 5:f:72:ASN:O      | 5:f:75:VAL:HG12   | 2.17                     | 0.44              |
| 7:h:80:THR:O      | 7:h:82:ILE:HG12   | 2.17                     | 0.44              |
| 17:r:75:VAL:HG22  | 17:r:86:GLN:CD    | 2.43                     | 0.44              |
| 18:s:13:SER:HB2   | 54:1:1266:G:O6    | 2.18                     | 0.44              |
| 19:t:38:ALA:HA    | 19:t:42:GLU:OE1   | 2.18                     | 0.44              |
| 22:w:74:LYS:HD3   | 22:w:74:LYS:N     | 2.33                     | 0.44              |
| 26:A:64:PHE:CZ    | 53:3:1011:C:H4'   | 2.53                     | 0.44              |
| 32:G:210:THR:HA   | 32:G:213:LEU:HD12 | 1.99                     | 0.44              |
| 34:I:12:ARG:NH2   | 34:I:31:CYS:HB2   | 2.33                     | 0.44              |
| 37:L:115:MET:O    | 37:L:119:LEU:HD23 | 2.18                     | 0.44              |
| 38:M:3:GLN:HG3    | 53:3:878:A:O4'    | 2.17                     | 0.44              |
| 38:M:9:MET:HG2    | 38:M:26:MET:CE    | 2.47                     | 0.44              |
| 38:M:124:ILE:HD11 | 38:M:127:TYR:CE1  | 2.52                     | 0.44              |
| 39:N:18:VAL:HG11  | 39:N:82:ILE:HD13  | 2.00                     | 0.44              |
| 44:S:69:PRO:HB3   | 53:3:981:U:O2'    | 2.17                     | 0.44              |
| 53:3:15:G:N2      | 53:3:1080:A:O2'   | 2.51                     | 0.44              |
| 53:3:434:U:H2'    | 53:3:435:A:C8     | 2.53                     | 0.44              |
| 53:3:823:C:H2'    | 53:3:824:G:C8     | 2.53                     | 0.44              |
| 53:3:1064:G:O3'   | 53:3:1065:U:H4'   | 2.18                     | 0.44              |
| 53:3:1164:G:N2    | 53:3:1165:U:C4    | 2.86                     | 0.44              |
| 54:1:161:A:N7     | 54:1:162:U:H5     | 2.16                     | 0.44              |
| 54:1:979:A:H2'    | 54:1:982:C:H42    | 1.82                     | 0.44              |
| 54:1:1149:G:H2'   | 54:1:1150:C:C6    | 2.53                     | 0.44              |
| 54:1:1507:C:H2'   | 54:1:1508:A:O4'   | 2.18                     | 0.44              |
| 54:1:2352:A:H2'   | 54:1:2353:G:H5'   | 1.98                     | 0.44              |
| 54:1:2457:U:H2'   | 54:1:2458:G:C8    | 2.53                     | 0.44              |
| 54:1:2580:U:C2'   | 54:1:2581:G:H5'   | 2.48                     | 0.44              |
| 54:1:2619:C:H2'   | 54:1:2620:C:C6    | 2.53                     | 0.44              |
| 54:1:2676:C:O2'   | 54:1:2677:G:H5'   | 2.18                     | 0.44              |
| 59:8:14:GLY:HA2   | 59:8:87:ILE:O     | 2.18                     | 0.44              |
| 1:b:216:ARG:NH2   | 54:1:781:A:OP1    | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:c:134:HIS:CE1   | 54:1:1675:C:C4    | 3.05                     | 0.44              |
| 5:f:34:ARG:HH21   | 54:1:2758:A:H2    | 1.66                     | 0.44              |
| 10:k:34:GLY:O     | 10:k:62:VAL:HB    | 2.17                     | 0.44              |
| 10:k:109:SER:C    | 10:k:111:LYS:H    | 2.26                     | 0.44              |
| 14:o:28:VAL:HG22  | 14:o:93:ASP:O     | 2.17                     | 0.44              |
| 16:q:57:ARG:O     | 16:q:61:ILE:HG12  | 2.18                     | 0.44              |
| 18:s:84:ARG:HH21  | 18:s:84:ARG:HG2   | 1.83                     | 0.44              |
| 34:I:95:GLY:HA3   | 34:I:135:GLN:OE1  | 2.17                     | 0.44              |
| 35:J:141:ASP:O    | 35:J:144:GLU:HB3  | 2.18                     | 0.44              |
| 42:Q:98:ARG:HB2   | 42:Q:116:TYR:HA   | 2.00                     | 0.44              |
| 48:W:11:ARG:HH21  | 53:3:845:A:H5'    | 1.83                     | 0.44              |
| 50:Y:23:ARG:HA    | 50:Y:23:ARG:NE    | 2.31                     | 0.44              |
| 51:Z:6:ARG:O      | 51:Z:7:GLU:HB2    | 2.18                     | 0.44              |
| 53:3:12:U:H2'     | 53:3:13:U:H5''    | 2.00                     | 0.44              |
| 53:3:532:A:P      | 53:3:532:A:H8     | 2.40                     | 0.44              |
| 53:3:1473:G:H2'   | 53:3:1474:U:C6    | 2.53                     | 0.44              |
| 54:1:96:C:H2'     | 54:1:97:C:C6      | 2.52                     | 0.44              |
| 54:1:1068:G:N2    | 54:1:1096:A:H5'   | 2.26                     | 0.44              |
| 54:1:1431:A:O2'   | 54:1:1432:G:H5'   | 2.17                     | 0.44              |
| 54:1:2324:U:O2'   | 54:1:2337:G:H5''  | 2.18                     | 0.44              |
| 56:5:11:C:H2'     | 56:5:12:G:C8      | 2.53                     | 0.44              |
| 59:8:79:TYR:HD2   | 59:8:80:GLU:HG2   | 1.82                     | 0.44              |
| 59:8:175:ALA:O    | 59:8:176:GLU:C    | 2.61                     | 0.44              |
| 59:8:222:LEU:C    | 59:8:222:LEU:HD23 | 2.43                     | 0.44              |
| 59:8:334:THR:HG23 | 59:8:385:ALA:HB3  | 1.99                     | 0.44              |
| 59:8:334:THR:O    | 59:8:385:ALA:N    | 2.51                     | 0.44              |
| 59:8:362:ARG:HD3  | 59:8:362:ARG:N    | 2.23                     | 0.44              |
| 4:e:32:LYS:HG2    | 4:e:91:ARG:NH1    | 2.32                     | 0.44              |
| 6:g:9:VAL:HG12    | 6:g:13:GLY:CA     | 2.47                     | 0.44              |
| 6:g:94:ILE:HD12   | 6:g:122:LEU:HD13  | 2.00                     | 0.44              |
| 12:m:53:MET:HG2   | 12:m:120:ALA:HB2  | 1.98                     | 0.44              |
| 21:v:38:LEU:CD2   | 21:v:40:ILE:HD11  | 2.48                     | 0.44              |
| 25:z:10:ARG:HG3   | 25:z:10:ARG:HH21  | 1.82                     | 0.44              |
| 27:B:42:ILE:HG22  | 27:B:48:TYR:HB2   | 2.00                     | 0.44              |
| 32:G:70:GLY:HA3   | 32:G:163:ILE:CG2  | 2.48                     | 0.44              |
| 32:G:131:LYS:HD2  | 53:3:1158:C:H1'   | 1.99                     | 0.44              |
| 34:I:84:ASN:O     | 34:I:88:ASN:ND2   | 2.47                     | 0.44              |
| 35:J:22:LYS:HA    | 53:3:1080:A:O3'   | 2.18                     | 0.44              |
| 40:O:7:ARG:HD2    | 53:3:1125:U:O4'   | 2.17                     | 0.44              |
| 41:P:12:ARG:HB2   | 41:P:13:LYS:HZ2   | 1.82                     | 0.44              |
| 41:P:115:ILE:HD12 | 41:P:115:ILE:N    | 2.33                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 43:R:73:SER:O    | 43:R:77:LYS:HG2   | 2.18                     | 0.44              |
| 46:U:1:MET:HG3   | 46:U:2:VAL:N      | 2.33                     | 0.44              |
| 48:W:47:ARG:HD2  | 48:W:47:ARG:N     | 2.33                     | 0.44              |
| 49:X:50:VAL:O    | 49:X:57:VAL:HG12  | 2.18                     | 0.44              |
| 53:3:163:C:H2'   | 53:3:164:G:O4'    | 2.17                     | 0.44              |
| 53:3:396:C:C2'   | 53:3:397:A:H5''   | 2.48                     | 0.44              |
| 53:3:538:G:H2'   | 53:3:539:A:C8     | 2.53                     | 0.44              |
| 53:3:620:C:H2'   | 53:3:621:A:O4'    | 2.18                     | 0.44              |
| 53:3:752:G:H4'   | 53:3:754:C:C5     | 2.53                     | 0.44              |
| 53:3:1000:A:H2'  | 53:3:1001:C:C6    | 2.53                     | 0.44              |
| 53:3:1217:C:H2'  | 53:3:1218:C:C6    | 2.52                     | 0.44              |
| 53:3:1356:G:O2'  | 53:3:1357:A:H5'   | 2.18                     | 0.44              |
| 53:3:1430:A:C2'  | 53:3:1431:A:H5'   | 2.48                     | 0.44              |
| 54:1:487:C:H2'   | 54:1:488:G:O4'    | 2.18                     | 0.44              |
| 54:1:609:A:H2'   | 54:1:610:C:O4'    | 2.18                     | 0.44              |
| 54:1:729:G:H2'   | 54:1:1775:U:H1'   | 1.99                     | 0.44              |
| 54:1:854:C:O2'   | 54:1:855:G:H5'    | 2.18                     | 0.44              |
| 54:1:1183:U:H2'  | 54:1:1184:U:C6    | 2.53                     | 0.44              |
| 54:1:1432:G:O2'  | 54:1:1433:A:H5'   | 2.17                     | 0.44              |
| 54:1:2028:U:H2'  | 54:1:2029:G:O4'   | 2.17                     | 0.44              |
| 54:1:2297:A:N6   | 54:1:2319:G:H1'   | 2.32                     | 0.44              |
| 54:1:2811:G:H2'  | 54:1:2812:G:C8    | 2.53                     | 0.44              |
| 59:8:120:GLN:HB2 | 59:8:161:ARG:NH2  | 2.33                     | 0.44              |
| 59:8:157:GLN:HA  | 59:8:160:THR:HG1  | 1.83                     | 0.44              |
| 1:b:14:HIS:O     | 1:b:203:VAL:HG21  | 2.18                     | 0.43              |
| 1:b:119:VAL:HG11 | 1:b:132:ARG:HH22  | 1.83                     | 0.43              |
| 1:b:204:LEU:HD23 | 54:1:1792:G:OP1   | 2.18                     | 0.43              |
| 4:e:72:SER:HB2   | 4:e:80:GLN:N      | 2.33                     | 0.43              |
| 5:f:97:VAL:C     | 5:f:98:LYS:HD3    | 2.43                     | 0.43              |
| 9:j:113:PRO:HD2  | 54:1:558:U:OP1    | 2.17                     | 0.43              |
| 10:k:76:VAL:H    | 15:p:72:VAL:CG2   | 2.30                     | 0.43              |
| 14:o:88:LYS:HG2  | 14:o:116:GLN:HB2  | 1.99                     | 0.43              |
| 17:r:6:GLN:CG    | 17:r:11:GLN:HE21  | 2.31                     | 0.43              |
| 32:G:96:LEU:HD11 | 53:3:1103:C:C5'   | 2.48                     | 0.43              |
| 32:G:113:LEU:CD2 | 32:G:151:LYS:HG3  | 2.47                     | 0.43              |
| 34:I:104:MET:HE1 | 34:I:172:VAL:CA   | 2.47                     | 0.43              |
| 35:J:21:SER:O    | 53:3:1080:A:H5''  | 2.17                     | 0.43              |
| 35:J:75:LEU:HD22 | 35:J:119:VAL:CG1  | 2.48                     | 0.43              |
| 37:L:30:MET:HE1  | 37:L:33:GLY:HA2   | 2.00                     | 0.43              |
| 39:N:3:ASN:O     | 39:N:21:LYS:HG2   | 2.18                     | 0.43              |
| 39:N:98:ARG:HH11 | 39:N:103:VAL:HG21 | 1.82                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 40:O:57:VAL:CG2  | 40:O:58:ASN:N     | 2.77                     | 0.43              |
| 43:R:92:ARG:NH1  | 43:R:92:ARG:CB    | 2.80                     | 0.43              |
| 50:Y:26:MET:C    | 50:Y:26:MET:SD    | 3.01                     | 0.43              |
| 52:a:42:VAL:HA   | 52:a:216:THR:HA   | 1.99                     | 0.43              |
| 53:3:21:G:H2'    | 53:3:22:G:H8      | 1.79                     | 0.43              |
| 53:3:403:C:O2'   | 53:3:404:G:H5'    | 2.18                     | 0.43              |
| 53:3:1122:U:C2'  | 53:3:1123:U:H5    | 2.31                     | 0.43              |
| 54:1:343:C:O2'   | 54:1:344:A:H5'    | 2.18                     | 0.43              |
| 54:1:532:A:H2'   | 54:1:532:A:N3     | 2.33                     | 0.43              |
| 54:1:634:C:H2'   | 54:1:635:C:C6     | 2.52                     | 0.43              |
| 54:1:799:G:C6    | 54:1:800:A:C6     | 3.06                     | 0.43              |
| 54:1:992:C:O2'   | 54:1:993:G:H5'    | 2.18                     | 0.43              |
| 54:1:1330:C:O2'  | 54:1:1331:G:H5'   | 2.17                     | 0.43              |
| 54:1:2512:C:H2'  | 54:1:2513:A:O4'   | 2.18                     | 0.43              |
| 59:8:190:ALA:HB3 | 59:8:206:ASP:O    | 2.17                     | 0.43              |
| 59:8:309:ARG:HD3 | 59:8:405:ILE:HG13 | 1.99                     | 0.43              |
| 59:8:521:ASP:HB2 | 59:8:577:ARG:HB2  | 1.99                     | 0.43              |
| 59:8:627:ASN:O   | 59:8:628:THR:C    | 2.60                     | 0.43              |
| 5:f:70:LEU:HD23  | 5:f:70:LEU:C      | 2.43                     | 0.43              |
| 10:k:64:ARG:HE   | 15:p:67:GLU:CD    | 2.26                     | 0.43              |
| 13:n:42:LYS:HE2  | 54:1:2818:U:OP2   | 2.18                     | 0.43              |
| 13:n:69:ARG:HG3  | 13:n:69:ARG:NH2   | 2.34                     | 0.43              |
| 15:p:8:GLU:OE1   | 15:p:54:LEU:HB3   | 2.18                     | 0.43              |
| 18:s:77:ASP:OD1  | 18:s:102:HIS:HB2  | 2.18                     | 0.43              |
| 20:u:4:ILE:H     | 20:u:4:ILE:CD1    | 2.28                     | 0.43              |
| 23:x:57:VAL:O    | 23:x:61:LYS:N     | 2.51                     | 0.43              |
| 26:A:36:VAL:HG21 | 26:A:41:HIS:HD2   | 1.83                     | 0.43              |
| 35:J:54:GLU:OE2  | 35:J:55:VAL:HG22  | 2.17                     | 0.43              |
| 38:M:44:PHE:O    | 38:M:45:ILE:HD13  | 2.18                     | 0.43              |
| 39:N:14:SER:HB2  | 39:N:69:GLY:HA3   | 1.99                     | 0.43              |
| 39:N:17:ARG:HH21 | 39:N:65:THR:HB    | 1.83                     | 0.43              |
| 40:O:40:ILE:CD1  | 40:O:73:LEU:HD12  | 2.47                     | 0.43              |
| 43:R:100:ARG:HG2 | 43:R:100:ARG:HH11 | 1.83                     | 0.43              |
| 44:S:52:ARG:HG2  | 44:S:58:ARG:HH11  | 1.84                     | 0.43              |
| 50:Y:66:ILE:CG2  | 50:Y:70:LYS:HB3   | 2.48                     | 0.43              |
| 52:a:40:GLU:N    | 52:a:178:VAL:HG22 | 2.33                     | 0.43              |
| 53:3:101:A:O2'   | 53:3:102:G:H5'    | 2.19                     | 0.43              |
| 53:3:930:C:O2'   | 53:3:931:C:H5'    | 2.18                     | 0.43              |
| 53:3:1053:G:H4'  | 53:3:1054:C:H3'   | 2.00                     | 0.43              |
| 54:1:207:A:C8    | 54:1:208:C:C5     | 3.06                     | 0.43              |
| 54:1:672:C:H2'   | 54:1:673:C:H6     | 1.83                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:1195:G:O2'   | 54:1:1196:C:H5'   | 2.18                     | 0.43              |
| 54:1:1285:A:H2'   | 54:1:1286:A:H5'   | 2.00                     | 0.43              |
| 54:1:1475:G:O2'   | 54:1:1476:U:H6    | 2.00                     | 0.43              |
| 54:1:1585:C:H2'   | 54:1:1586:A:O4'   | 2.17                     | 0.43              |
| 54:1:2194:U:H2'   | 54:1:2195:U:H6    | 1.83                     | 0.43              |
| 54:1:2373:G:H2'   | 54:1:2374:C:H6    | 1.83                     | 0.43              |
| 54:1:2588:G:C2'   | 54:1:2589:A:H5'   | 2.48                     | 0.43              |
| 54:1:2727:A:H2'   | 54:1:2728:U:C6    | 2.53                     | 0.43              |
| 54:1:2814:A:H2'   | 54:1:2815:C:H6    | 1.83                     | 0.43              |
| 55:2:87:U:H5''    | 55:2:88:C:OP2     | 2.18                     | 0.43              |
| 59:8:505:HIS:CE1  | 59:8:595:LEU:HD12 | 2.53                     | 0.43              |
| 11:l:21:ARG:HH21  | 11:l:21:ARG:HG2   | 1.82                     | 0.43              |
| 11:l:38:GLN:HE21  | 54:1:805:G:C1'    | 2.31                     | 0.43              |
| 11:l:64:PHE:CZ    | 30:E:14:LYS:HD3   | 2.53                     | 0.43              |
| 14:o:64:TYR:O     | 14:o:67:ASN:ND2   | 2.51                     | 0.43              |
| 19:t:23:ALA:O     | 19:t:28:ASN:N     | 2.50                     | 0.43              |
| 20:u:73:ASN:O     | 20:u:74:ALA:HB3   | 2.18                     | 0.43              |
| 32:G:134:LEU:HD12 | 32:G:134:LEU:C    | 2.43                     | 0.43              |
| 36:K:44:ARG:HB2   | 36:K:58:HIS:CE1   | 2.53                     | 0.43              |
| 39:N:39:GLY:C     | 39:N:44:ARG:HB2   | 2.43                     | 0.43              |
| 42:Q:98:ARG:HH12  | 42:Q:106:VAL:HG22 | 1.81                     | 0.43              |
| 46:U:38:PHE:CE1   | 46:U:51:ARG:HB3   | 2.53                     | 0.43              |
| 46:U:42:ILE:HG13  | 46:U:43:ALA:N     | 2.33                     | 0.43              |
| 53:3:406:G:O2'    | 53:3:407:U:H5'    | 2.19                     | 0.43              |
| 53:3:1217:C:H2'   | 53:3:1218:C:O4'   | 2.19                     | 0.43              |
| 53:3:1304:G:H21   | 53:3:1333:A:H62   | 1.66                     | 0.43              |
| 53:3:1309:G:C6    | 53:3:1329:A:C2    | 3.06                     | 0.43              |
| 54:1:194:G:C2     | 54:1:202:U:H1'    | 2.53                     | 0.43              |
| 54:1:1186:G:H2'   | 54:1:1187:G:O4'   | 2.18                     | 0.43              |
| 54:1:1486:U:H2'   | 54:1:1487:U:C6    | 2.53                     | 0.43              |
| 54:1:2130:U:O3'   | 54:1:2134:A:H5'   | 2.17                     | 0.43              |
| 54:1:2372:U:H2'   | 54:1:2373:G:C8    | 2.52                     | 0.43              |
| 55:2:28:C:H2'     | 55:2:29:A:H8      | 1.81                     | 0.43              |
| 57:6:70:G:H2'     | 57:6:71:C:C6      | 2.53                     | 0.43              |
| 59:8:347:ASP:H    | 59:8:360:PHE:HB2  | 1.82                     | 0.43              |
| 4:e:31:GLU:O      | 4:e:91:ARG:HG3    | 2.18                     | 0.43              |
| 4:e:37:MET:SD     | 4:e:151:LEU:HB3   | 2.58                     | 0.43              |
| 5:f:13:GLY:HA3    | 5:f:28:LYS:HZ1    | 1.83                     | 0.43              |
| 7:h:43:LYS:O      | 7:h:46:ARG:HB3    | 2.18                     | 0.43              |
| 8:i:11:GLN:O      | 8:i:54:ILE:O      | 2.35                     | 0.43              |
| 10:k:14:SER:OG    | 10:k:86:LEU:HD12  | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:o:34:HIS:CE1   | 14:o:54:VAL:HA    | 2.53                     | 0.43              |
| 15:p:87:ARG:HG3   | 15:p:87:ARG:HH11  | 1.84                     | 0.43              |
| 15:p:102:ARG:HG2  | 15:p:102:ARG:NH1  | 2.33                     | 0.43              |
| 16:q:87:VAL:HG12  | 16:q:89:ILE:H     | 1.82                     | 0.43              |
| 24:y:16:THR:O     | 24:y:19:LEU:HB2   | 2.18                     | 0.43              |
| 34:I:204:SER:HB2  | 53:3:8:A:H62      | 1.83                     | 0.43              |
| 35:J:104:ILE:HG23 | 35:J:111:ARG:NH1  | 2.32                     | 0.43              |
| 38:M:17:GLN:OE1   | 38:M:17:GLN:HA    | 2.18                     | 0.43              |
| 40:O:7:ARG:C      | 40:O:8:ILE:HD12   | 2.43                     | 0.43              |
| 40:O:11:LYS:HB3   | 40:O:71:LEU:HA    | 1.99                     | 0.43              |
| 41:P:124:LYS:O    | 51:Z:34:ARG:CZ    | 2.67                     | 0.43              |
| 42:Q:110:LYS:HB2  | 42:Q:111:GLN:OE1  | 2.18                     | 0.43              |
| 43:R:7:ASN:CG     | 43:R:9:PRO:HD3    | 2.43                     | 0.43              |
| 43:R:76:ILE:HA    | 43:R:79:LEU:CD2   | 2.48                     | 0.43              |
| 44:S:20:PHE:CE1   | 44:S:27:LYS:HG2   | 2.54                     | 0.43              |
| 49:X:32:THR:O     | 49:X:50:VAL:HA    | 2.18                     | 0.43              |
| 50:Y:81:GLN:O     | 50:Y:84:LYS:HB3   | 2.18                     | 0.43              |
| 52:a:11:ILE:HD13  | 52:a:218:MET:O    | 2.17                     | 0.43              |
| 53:3:20:U:H2'     | 53:3:21:G:O4'     | 2.17                     | 0.43              |
| 53:3:186:C:H2'    | 53:3:187:G:O4'    | 2.18                     | 0.43              |
| 53:3:253:A:N6     | 53:3:274:A:N1     | 2.66                     | 0.43              |
| 53:3:499:A:O4'    | 53:3:547:A:N6     | 2.51                     | 0.43              |
| 53:3:538:G:O2'    | 53:3:539:A:H5'    | 2.19                     | 0.43              |
| 53:3:1033:G:H2'   | 53:3:1034:G:C5'   | 2.35                     | 0.43              |
| 53:3:1091:U:H4'   | 53:3:1172:C:OP1   | 2.17                     | 0.43              |
| 54:1:728:G:C4     | 54:1:730:A:C8     | 3.06                     | 0.43              |
| 54:1:772:C:H2'    | 54:1:773:U:C6     | 2.54                     | 0.43              |
| 54:1:1549:A:H2'   | 54:1:1550:C:H6    | 1.81                     | 0.43              |
| 54:1:1611:C:H6    | 54:1:1611:C:H5'   | 1.83                     | 0.43              |
| 54:1:1688:U:H2'   | 54:1:1698:A:N6    | 2.33                     | 0.43              |
| 54:1:1890:A:H2'   | 54:1:1891:G:H8    | 1.83                     | 0.43              |
| 54:1:1904:G:N2    | 54:1:1905:C:H1'   | 2.33                     | 0.43              |
| 54:1:2019:A:H2'   | 54:1:2020:A:H5''  | 2.00                     | 0.43              |
| 54:1:2128:G:H2'   | 54:1:2129:C:O5'   | 2.18                     | 0.43              |
| 54:1:2580:U:H2'   | 54:1:2581:G:H5'   | 2.00                     | 0.43              |
| 54:1:2638:G:H1'   | 54:1:2778:A:N6    | 2.33                     | 0.43              |
| 54:1:2646:C:H2'   | 54:1:2647:U:O4'   | 2.19                     | 0.43              |
| 59:8:167:VAL:O    | 59:8:167:VAL:HG23 | 2.17                     | 0.43              |
| 59:8:388:LEU:HD23 | 59:8:391:VAL:HG11 | 2.00                     | 0.43              |
| 1:b:76:VAL:HG22   | 1:b:114:GLN:HB3   | 2.00                     | 0.43              |
| 1:b:119:VAL:HG23  | 6:g:91:PHE:CE1    | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:b:218:THR:O     | 54:1:1789:A:H5''  | 2.17                     | 0.43              |
| 2:c:49:GLN:NE2    | 2:c:79:LEU:HD13   | 2.33                     | 0.43              |
| 11:l:32:GLY:HA2   | 54:1:1190:G:H5''  | 1.99                     | 0.43              |
| 12:m:35:ALA:HA    | 12:m:128:THR:HA   | 2.00                     | 0.43              |
| 14:o:111:ARG:HH21 | 14:o:111:ARG:HG3  | 1.83                     | 0.43              |
| 22:w:50:GLY:C     | 22:w:52:ASP:H     | 2.27                     | 0.43              |
| 32:G:63:LYS:HD3   | 32:G:63:LYS:N     | 2.34                     | 0.43              |
| 34:I:196:GLU:O    | 34:I:200:VAL:HG23 | 2.18                     | 0.43              |
| 35:J:24:VAL:HG12  | 35:J:29:ILE:HG13  | 2.01                     | 0.43              |
| 36:K:4:TYR:CD2    | 36:K:71:ILE:HG13  | 2.54                     | 0.43              |
| 36:K:13:ASP:OD1   | 36:K:13:ASP:N     | 2.50                     | 0.43              |
| 37:L:94:ARG:O     | 37:L:98:LEU:HD13  | 2.19                     | 0.43              |
| 39:N:24:ASN:O     | 39:N:61:ASP:HB3   | 2.18                     | 0.43              |
| 40:O:39:PRO:HB3   | 53:3:1123:U:C5    | 2.52                     | 0.43              |
| 42:Q:32:VAL:CG2   | 42:Q:55:ARG:HB3   | 2.48                     | 0.43              |
| 49:X:71:GLY:HA3   | 53:3:1320:C:H1'   | 2.01                     | 0.43              |
| 51:Z:39:LYS:N     | 51:Z:40:PRO:CD    | 2.82                     | 0.43              |
| 52:a:39:VAL:HG11  | 52:a:177:LYS:HB3  | 2.00                     | 0.43              |
| 53:3:427:U:H3'    | 53:3:428:G:H2'    | 1.99                     | 0.43              |
| 53:3:952:U:C5'    | 53:3:972:C:H41    | 2.30                     | 0.43              |
| 53:3:1389:C:H2'   | 53:3:1390:U:H5'   | 1.99                     | 0.43              |
| 54:1:418:C:H2'    | 54:1:419:U:C6     | 2.53                     | 0.43              |
| 54:1:679:C:O2'    | 54:1:680:C:H5'    | 2.19                     | 0.43              |
| 54:1:724:U:H2'    | 54:1:725:G:O4'    | 2.18                     | 0.43              |
| 54:1:800:A:C2     | 54:1:802:A:C8     | 3.07                     | 0.43              |
| 54:1:1077:A:C2'   | 54:1:1078:U:H5'   | 2.48                     | 0.43              |
| 54:1:1197:G:H2'   | 54:1:1198:U:H6    | 1.82                     | 0.43              |
| 54:1:2135:A:O2'   | 54:1:2160:C:H5'   | 2.18                     | 0.43              |
| 54:1:2686:G:H2'   | 54:1:2687:U:O4'   | 2.18                     | 0.43              |
| 55:2:21:G:O2'     | 55:2:22:U:H5'     | 2.18                     | 0.43              |
| 55:2:28:C:H2'     | 55:2:29:A:C8      | 2.53                     | 0.43              |
| 55:2:63:C:H2'     | 55:2:64:G:H8      | 1.83                     | 0.43              |
| 59:8:11:ARG:HG3   | 59:8:11:ARG:NH1   | 2.34                     | 0.43              |
| 59:8:119:VAL:O    | 59:8:123:SER:HB3  | 2.18                     | 0.43              |
| 59:8:223:ILE:HA   | 59:8:226:ALA:HB2  | 2.01                     | 0.43              |
| 59:8:364:VAL:HG23 | 59:8:372:GLU:C    | 2.43                     | 0.43              |
| 59:8:498:VAL:HA   | 59:8:607:LYS:NZ   | 2.34                     | 0.43              |
| 1:b:94:LEU:HD12   | 1:b:94:LEU:O      | 2.19                     | 0.43              |
| 2:c:47:ALA:HA     | 2:c:84:LEU:HG     | 2.01                     | 0.43              |
| 5:f:132:LEU:C     | 5:f:132:LEU:HD12  | 2.44                     | 0.43              |
| 6:g:9:VAL:HG22    | 6:g:10:ALA:N      | 2.33                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 7:h:80:THR:O    | 7:h:81:LEU:C     | 2.62                     | 0.43              |
| 8:i:4:VAL:HG13  | 8:i:7:TYR:HE1    | 1.83                     | 0.43              |
| 9:j:2:LYS:HD3   | 54:1:995:C:N4    | 2.32                     | 0.43              |
| 9:j:81:ILE:HG23 | 9:j:82:GLY:N     | 2.33                     | 0.43              |
| 11:l:47:ARG:HE  | 54:1:251:A:H5''  | 1.82                     | 0.43              |
| 13:n:69:ARG:C   | 13:n:71:ARG:H    | 2.27                     | 0.43              |
| 16:q:55:GLN:O   | 16:q:58:GLN:HB2  | 2.18                     | 0.43              |
| 17:r:61:ALA:HB2 | 17:r:98:ILE:HD13 | 2.00                     | 0.43              |
| 20:u:36:GLU:O   | 20:u:38:ILE:HG12 | 2.18                     | 0.43              |
| 21:v:39:ALA:O   | 21:v:40:ILE:HD13 | 2.18                     | 0.43              |
| 21:v:47:VAL:HA  | 21:v:50:MET:HE2  | 2.00                     | 0.43              |
| 35:J:64:GLU:CD  | 35:J:64:GLU:N    | 2.75                     | 0.43              |
| 36:K:6:ILE:HG23 | 36:K:62:MET:HB2  | 1.99                     | 0.43              |
| 39:N:48:ARG:O   | 39:N:52:GLU:HG2  | 2.19                     | 0.43              |
| 40:O:83:THR:O   | 40:O:87:LEU:HG   | 2.19                     | 0.43              |
| 40:O:88:MET:C   | 40:O:90:LEU:H    | 2.27                     | 0.43              |
| 44:S:88:MET:N   | 44:S:88:MET:SD   | 2.91                     | 0.43              |
| 46:U:41:PRO:HG2 | 46:U:42:ILE:H    | 1.84                     | 0.43              |
| 46:U:77:GLU:O   | 46:U:79:ASN:OD1  | 2.37                     | 0.43              |
| 53:3:218:U:H2'  | 53:3:219:U:O4'   | 2.18                     | 0.43              |
| 53:3:451:A:H4'  | 53:3:452:A:O4'   | 2.18                     | 0.43              |
| 53:3:958:A:H2   | 53:3:986:U:H1'   | 1.83                     | 0.43              |
| 53:3:1053:G:N7  | 53:3:1199:U:H2'  | 2.33                     | 0.43              |
| 53:3:1346:A:H2' | 53:3:1346:A:N3   | 2.34                     | 0.43              |
| 53:3:1360:A:H2' | 53:3:1361:G:C5'  | 2.49                     | 0.43              |
| 54:1:819:A:C4   | 54:1:1189:A:C2   | 3.07                     | 0.43              |
| 54:1:932:U:H6   | 54:1:932:U:OP1   | 2.01                     | 0.43              |
| 54:1:936:A:H2'  | 54:1:937:C:C6    | 2.52                     | 0.43              |
| 54:1:1047:G:H2' | 54:1:1110:G:N1   | 2.33                     | 0.43              |
| 54:1:1798:U:C4  | 54:1:1819:A:C2   | 3.07                     | 0.43              |
| 55:2:32:U:H2'   | 55:2:33:G:C8     | 2.53                     | 0.43              |
| 56:5:59:A:C2'   | 56:5:60:U:H5'    | 2.48                     | 0.43              |
| 59:8:350:LEU:H  | 59:8:399:ASP:HA  | 1.84                     | 0.43              |
| 2:c:33:ARG:HH22 | 2:c:74:GLU:HB3   | 1.83                     | 0.43              |
| 2:c:98:VAL:HG22 | 2:c:98:VAL:O     | 2.18                     | 0.43              |
| 4:e:7:TYR:HD1   | 4:e:11:VAL:HG21  | 1.83                     | 0.43              |
| 7:h:14:GLU:OE1  | 7:h:66:GLY:HA3   | 2.19                     | 0.43              |
| 7:h:58:THR:HG21 | 7:h:82:ILE:H     | 1.83                     | 0.43              |
| 8:i:71:LYS:HE3  | 54:1:1060:U:OP2  | 2.19                     | 0.43              |
| 9:j:34:ARG:HH11 | 9:j:34:ARG:HG3   | 1.82                     | 0.43              |
| 10:k:64:ARG:NE  | 15:p:67:GLU:OE2  | 2.45                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:u:17:ASP:HB3   | 20:u:20:LYS:HD2   | 2.00                     | 0.43              |
| 22:w:37:ARG:NH1   | 54:1:2387:U:H4'   | 2.33                     | 0.43              |
| 29:D:29:GLN:HB3   | 29:D:33:ARG:HH22  | 1.84                     | 0.43              |
| 32:G:80:LYS:HG3   | 32:G:90:PHE:CE2   | 2.53                     | 0.43              |
| 33:H:122:GLN:O    | 33:H:127:VAL:HG12 | 2.18                     | 0.43              |
| 33:H:142:ARG:CB   | 33:H:142:ARG:NH1  | 2.81                     | 0.43              |
| 41:P:51:PHE:HB3   | 41:P:55:ARG:CB    | 2.46                     | 0.43              |
| 41:P:92:ARG:HE    | 51:Z:24:LYS:HZ1   | 1.65                     | 0.43              |
| 46:U:37:GLY:HA3   | 46:U:52:LEU:HA    | 2.00                     | 0.43              |
| 47:V:6:THR:C      | 47:V:7:LEU:HD12   | 2.43                     | 0.43              |
| 53:3:192:A:H2'    | 53:3:193:C:O4'    | 2.19                     | 0.43              |
| 53:3:319:G:O2'    | 53:3:320:A:H5'    | 2.19                     | 0.43              |
| 53:3:460:A:H2'    | 53:3:461:A:C8     | 2.53                     | 0.43              |
| 53:3:553:A:H2'    | 53:3:554:A:C8     | 2.54                     | 0.43              |
| 53:3:814:A:H5''   | 53:3:816:A:N7     | 2.33                     | 0.43              |
| 54:1:395:U:H2'    | 54:1:396:G:C8     | 2.53                     | 0.43              |
| 54:1:825:A:H2'    | 54:1:826:U:C6     | 2.54                     | 0.43              |
| 54:1:934:U:H2'    | 54:1:935:C:H6     | 1.83                     | 0.43              |
| 54:1:1213:A:H2'   | 54:1:1214:A:C8    | 2.53                     | 0.43              |
| 54:1:1625:C:H2'   | 54:1:1626:A:O4'   | 2.18                     | 0.43              |
| 54:1:1788:C:H2'   | 54:1:1789:A:C8    | 2.51                     | 0.43              |
| 54:1:2055:C:H2'   | 54:1:2504:U:H5'   | 2.00                     | 0.43              |
| 54:1:2418:A:H2'   | 54:1:2419:U:O4'   | 2.18                     | 0.43              |
| 59:8:86:ILE:HG23  | 59:8:86:ILE:O     | 2.18                     | 0.43              |
| 59:8:453:SER:HB2  | 59:8:487:GLN:HG3  | 2.01                     | 0.43              |
| 59:8:520:ILE:HB   | 59:8:576:ILE:HD11 | 2.00                     | 0.43              |
| 59:8:526:GLU:C    | 59:8:528:GLY:H    | 2.26                     | 0.43              |
| 1:b:175:LEU:HD13  | 54:1:1799:G:C4    | 2.53                     | 0.43              |
| 4:e:115:GLY:CA    | 4:e:177:ARG:HB2   | 2.43                     | 0.43              |
| 7:h:14:GLU:O      | 7:h:18:VAL:HG23   | 2.18                     | 0.43              |
| 10:k:93:GLN:OE1   | 10:k:93:GLN:N     | 2.50                     | 0.43              |
| 11:l:121:THR:HG23 | 11:l:141:LYS:HG3  | 2.01                     | 0.43              |
| 14:o:35:ILE:HD13  | 14:o:71:ALA:HB1   | 2.00                     | 0.43              |
| 19:t:8:LEU:HD13   | 24:y:21:LEU:CB    | 2.48                     | 0.43              |
| 20:u:46:LYS:HD2   | 20:u:46:LYS:C     | 2.44                     | 0.43              |
| 26:A:42:PRO:HA    | 26:A:44:PHE:CE1   | 2.54                     | 0.43              |
| 26:A:57:VAL:O     | 26:A:60:PHE:HB3   | 2.19                     | 0.43              |
| 28:C:9:LYS:C      | 28:C:10:LEU:HD12  | 2.43                     | 0.43              |
| 29:D:12:ARG:CZ    | 29:D:44:VAL:HG21  | 2.49                     | 0.43              |
| 32:G:44:LYS:O     | 32:G:48:MET:HG2   | 2.19                     | 0.43              |
| 34:I:97:LEU:O     | 34:I:101:VAL:HG23 | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:N:98:ARG:HG3   | 39:N:103:VAL:CG2  | 2.40                     | 0.43              |
| 40:O:11:LYS:HB3   | 40:O:71:LEU:HG    | 2.01                     | 0.43              |
| 40:O:49:PHE:CE2   | 44:S:76:PHE:HZ    | 2.37                     | 0.43              |
| 44:S:27:LYS:C     | 44:S:27:LYS:CD    | 2.92                     | 0.43              |
| 45:T:55:LEU:HD21  | 54:1:715:A:C2     | 2.54                     | 0.43              |
| 46:U:73:ALA:O     | 46:U:77:GLU:N     | 2.45                     | 0.43              |
| 48:W:12:PHE:C     | 48:W:14:ALA:N     | 2.76                     | 0.43              |
| 53:3:233:C:H2'    | 53:3:234:C:C6     | 2.53                     | 0.43              |
| 53:3:1079:G:HO2'  | 53:3:1080:A:H5'   | 1.78                     | 0.43              |
| 53:3:1256:A:H1'   | 53:3:1258:G:C4    | 2.54                     | 0.43              |
| 53:3:1425:U:O2'   | 53:3:1426:G:H5'   | 2.18                     | 0.43              |
| 53:3:1523:G:C6    | 53:3:1524:C:N4    | 2.87                     | 0.43              |
| 54:1:572:A:H5''   | 54:1:573:U:OP2    | 2.19                     | 0.43              |
| 54:1:708:G:H2'    | 54:1:709:U:H6     | 1.84                     | 0.43              |
| 54:1:856:G:H2'    | 54:1:857:G:C8     | 2.54                     | 0.43              |
| 54:1:927:A:H2'    | 54:1:928:A:C8     | 2.54                     | 0.43              |
| 54:1:1775:U:H2'   | 54:1:1776:G:C5'   | 2.44                     | 0.43              |
| 54:1:2743:U:H2'   | 54:1:2744:G:C5'   | 2.45                     | 0.43              |
| 57:6:46:G:C2'     | 57:6:47:U:H5'     | 2.47                     | 0.43              |
| 59:8:68:THR:HG22  | 59:8:69:THR:H     | 1.84                     | 0.43              |
| 59:8:342:VAL:HG11 | 59:8:378:ARG:HH11 | 1.83                     | 0.43              |
| 5:f:46:ASP:CG     | 5:f:47:ASN:N      | 2.72                     | 0.43              |
| 7:h:40:GLU:O      | 7:h:44:ALA:N      | 2.46                     | 0.43              |
| 10:k:25:LEU:HD23  | 10:k:39:ILE:CA    | 2.49                     | 0.43              |
| 12:m:132:THR:HG22 | 12:m:133:LYS:N    | 2.34                     | 0.43              |
| 13:n:12:ARG:HH21  | 13:n:12:ARG:CB    | 2.32                     | 0.43              |
| 21:v:10:LYS:HG3   | 21:v:11:GLU:N     | 2.34                     | 0.43              |
| 21:v:20:LEU:HD12  | 21:v:20:LEU:C     | 2.43                     | 0.43              |
| 21:v:75:GLN:HB2   | 21:v:92:VAL:HG12  | 2.01                     | 0.43              |
| 23:x:11:PRO:HA    | 23:x:28:PHE:O     | 2.19                     | 0.43              |
| 34:I:150:LYS:HZ2  | 34:I:155:LYS:HA   | 1.84                     | 0.43              |
| 34:I:187:ARG:CZ   | 34:I:192:ALA:HA   | 2.49                     | 0.43              |
| 37:L:53:SER:OG    | 37:L:55:LYS:HG2   | 2.19                     | 0.43              |
| 39:N:53:LEU:HD12  | 39:N:53:LEU:N     | 2.34                     | 0.43              |
| 39:N:123:ARG:HB3  | 53:3:1343:G:O3'   | 2.19                     | 0.43              |
| 43:R:79:LEU:CD1   | 43:R:87:GLY:HA2   | 2.49                     | 0.43              |
| 43:R:92:ARG:HB2   | 43:R:92:ARG:CZ    | 2.48                     | 0.43              |
| 43:R:106:ARG:HE   | 43:R:109:LYS:HD3  | 1.84                     | 0.43              |
| 52:a:65:LEU:O     | 52:a:159:GLY:HA3  | 2.18                     | 0.43              |
| 53:3:260:G:H2'    | 53:3:261:U:C6     | 2.54                     | 0.43              |
| 53:3:297:G:H4'    | 53:3:557:G:H4'    | 2.01                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 53:3:1200:C:H4'   | 53:3:1201:A:H3'  | 2.01                     | 0.43              |
| 53:3:1216:A:O2'   | 53:3:1217:C:H5'  | 2.19                     | 0.43              |
| 53:3:1269:A:C2    | 53:3:1313:U:O4'  | 2.72                     | 0.43              |
| 53:3:1328:C:N4    | 53:3:1329:A:N6   | 2.66                     | 0.43              |
| 54:1:224:U:H2'    | 54:1:225:C:O4'   | 2.19                     | 0.43              |
| 54:1:399:U:OP1    | 54:1:2090:A:H5'' | 2.18                     | 0.43              |
| 54:1:566:U:H2'    | 54:1:567:U:O4'   | 2.18                     | 0.43              |
| 54:1:1176:U:H2'   | 54:1:1177:G:N9   | 2.34                     | 0.43              |
| 54:1:1344:U:H4'   | 54:1:1384:A:C5   | 2.54                     | 0.43              |
| 54:1:1820:U:H4'   | 54:1:1821:A:OP2  | 2.18                     | 0.43              |
| 54:1:2065:C:H1'   | 54:1:2449:U:N3   | 2.34                     | 0.43              |
| 54:1:2287:A:C5    | 54:1:2289:G:C8   | 3.06                     | 0.43              |
| 54:1:2709:G:H2'   | 54:1:2710:C:C6   | 2.54                     | 0.43              |
| 54:1:2716:C:C2'   | 54:1:2717:C:H5'  | 2.49                     | 0.43              |
| 56:5:1:C:H2'      | 56:5:2:G:H8      | 1.83                     | 0.43              |
| 59:8:104:ARG:HG2  | 59:8:104:ARG:NH1 | 2.34                     | 0.43              |
| 59:8:218:TRP:O    | 59:8:222:LEU:N   | 2.47                     | 0.43              |
| 59:8:327:ASP:N    | 59:8:331:GLY:O   | 2.50                     | 0.43              |
| 59:8:624:PRO:O    | 59:8:650:THR:O   | 2.37                     | 0.43              |
| 1:b:104:LEU:CD1   | 1:b:155:ARG:HG2  | 2.49                     | 0.43              |
| 4:e:116:LEU:O     | 4:e:177:ARG:N    | 2.50                     | 0.43              |
| 7:h:57:ASN:HB2    | 7:h:62:ARG:CD    | 2.37                     | 0.43              |
| 10:k:22:ILE:HG13  | 10:k:23:LYS:H    | 1.84                     | 0.43              |
| 34:I:104:MET:HE2  | 34:I:179:GLY:CA  | 2.45                     | 0.43              |
| 35:J:163:ILE:HG13 | 35:J:164:LEU:N   | 2.34                     | 0.43              |
| 37:L:16:LYS:HG2   | 37:L:17:PHE:HD1  | 1.82                     | 0.43              |
| 38:M:17:GLN:OE1   | 38:M:62:LEU:HD13 | 2.19                     | 0.43              |
| 38:M:35:ILE:HG13  | 38:M:36:ALA:N    | 2.33                     | 0.43              |
| 39:N:27:ILE:HG22  | 39:N:29:ILE:HD11 | 2.00                     | 0.43              |
| 41:P:31:VAL:CG1   | 41:P:44:ALA:HB3  | 2.48                     | 0.43              |
| 43:R:95:PRO:HD3   | 43:R:108:ARG:HD2 | 2.01                     | 0.43              |
| 46:U:20:VAL:CG2   | 46:U:21:VAL:N    | 2.82                     | 0.43              |
| 53:3:536:C:C2'    | 53:3:537:G:H5'   | 2.49                     | 0.43              |
| 53:3:599:C:H2'    | 53:3:600:A:H8    | 1.84                     | 0.43              |
| 53:3:633:G:H2'    | 53:3:634:C:C6    | 2.54                     | 0.43              |
| 53:3:806:C:H2'    | 53:3:807:A:H8    | 1.84                     | 0.43              |
| 53:3:865:A:H2'    | 53:3:866:C:C6    | 2.53                     | 0.43              |
| 53:3:1251:A:H1'   | 53:3:1370:G:C4'  | 2.49                     | 0.43              |
| 54:1:281:C:H2'    | 54:1:282:A:H8    | 1.83                     | 0.43              |
| 54:1:632:A:H2'    | 54:1:633:A:C8    | 2.53                     | 0.43              |
| 54:1:694:U:H3'    | 54:1:695:G:H5''  | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:725:G:C6     | 54:1:726:G:N1     | 2.87                     | 0.43              |
| 54:1:1023:U:H4'   | 54:1:1123:C:OP1   | 2.17                     | 0.43              |
| 54:1:1572:A:H2'   | 54:1:1573:G:C8    | 2.53                     | 0.43              |
| 54:1:2842:G:O2'   | 54:1:2843:G:H5'   | 2.18                     | 0.43              |
| 57:6:62:C:H2'     | 57:6:63:G:H8      | 1.83                     | 0.43              |
| 59:8:52:TRP:CD1   | 59:8:369:ASN:HD21 | 2.37                     | 0.43              |
| 59:8:170:GLN:OE1  | 59:8:170:GLN:HA   | 2.19                     | 0.43              |
| 59:8:236:LYS:CG   | 59:8:243:LEU:HD21 | 2.44                     | 0.43              |
| 59:8:633:GLY:O    | 59:8:637:ARG:HG3  | 2.19                     | 0.43              |
| 1:b:73:ILE:HG23   | 54:1:1490:A:H62   | 1.84                     | 0.42              |
| 1:b:204:LEU:CD1   | 1:b:213:ARG:HH21  | 2.32                     | 0.42              |
| 2:c:4:LEU:HD23    | 2:c:29:VAL:HG11   | 2.00                     | 0.42              |
| 2:c:46:ARG:HG3    | 2:c:84:LEU:HB2    | 2.01                     | 0.42              |
| 3:d:104:ALA:O     | 3:d:108:ILE:HG13  | 2.18                     | 0.42              |
| 6:g:103:VAL:HG12  | 6:g:108:VAL:O     | 2.19                     | 0.42              |
| 7:h:41:LEU:HD13   | 54:1:1083:U:H4'   | 2.01                     | 0.42              |
| 17:r:6:GLN:NE2    | 17:r:11:GLN:NE2   | 2.67                     | 0.42              |
| 18:s:75:PHE:CE1   | 18:s:104:THR:HB   | 2.54                     | 0.42              |
| 18:s:83:LYS:HG2   | 18:s:95:ARG:NH1   | 2.23                     | 0.42              |
| 31:F:15:LYS:O     | 31:F:25:VAL:HA    | 2.19                     | 0.42              |
| 40:O:72:ARG:HA    | 40:O:72:ARG:HD3   | 1.90                     | 0.42              |
| 41:P:34:THR:OG1   | 41:P:35:ASP:N     | 2.51                     | 0.42              |
| 43:R:82:LEU:HD23  | 43:R:84:CYS:HB3   | 2.01                     | 0.42              |
| 43:R:106:ARG:NH1  | 43:R:112:ARG:HH21 | 2.17                     | 0.42              |
| 47:V:45:VAL:HG13  | 47:V:72:TRP:C     | 2.43                     | 0.42              |
| 50:Y:73:ARG:O     | 50:Y:77:ASN:ND2   | 2.52                     | 0.42              |
| 52:a:42:VAL:HG13  | 52:a:215:SER:O    | 2.19                     | 0.42              |
| 53:3:224:U:H2'    | 53:3:225:C:H6     | 1.80                     | 0.42              |
| 53:3:295:C:H2'    | 53:3:296:U:O4'    | 2.19                     | 0.42              |
| 53:3:332:G:O2'    | 53:3:333:U:H5'    | 2.20                     | 0.42              |
| 53:3:730:G:O2'    | 53:3:766:A:H5'    | 2.18                     | 0.42              |
| 54:1:460:A:H1'    | 54:1:470:A:N6     | 2.34                     | 0.42              |
| 54:1:597:G:H2'    | 54:1:598:U:C6     | 2.54                     | 0.42              |
| 54:1:600:G:H2'    | 54:1:601:C:C6     | 2.54                     | 0.42              |
| 54:1:1541:C:H2'   | 54:1:1542:U:C6    | 2.53                     | 0.42              |
| 54:1:1748:C:H2'   | 54:1:1749:A:H8    | 1.83                     | 0.42              |
| 54:1:1854:A:H2    | 54:1:2088:A:O4'   | 2.02                     | 0.42              |
| 59:8:320:LEU:HD23 | 59:8:320:LEU:C    | 2.44                     | 0.42              |
| 8:i:56:VAL:HG22   | 8:i:57:VAL:N      | 2.34                     | 0.42              |
| 10:k:104:THR:HG22 | 10:k:105:ARG:N    | 2.34                     | 0.42              |
| 13:n:100:CYS:SG   | 13:n:101:GLY:N    | 2.92                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 13:n:117:ASP:CG   | 13:n:118:ARG:H   | 2.23                     | 0.42              |
| 17:r:14:VAL:HG21  | 17:r:98:ILE:HG13 | 2.01                     | 0.42              |
| 18:s:20:VAL:HG11  | 18:s:47:VAL:HG11 | 2.01                     | 0.42              |
| 18:s:88:ARG:HG3   | 18:s:88:ARG:HH21 | 1.84                     | 0.42              |
| 20:u:81:ARG:NH2   | 20:u:81:ARG:HG2  | 2.33                     | 0.42              |
| 21:v:28:ALA:N     | 21:v:40:ILE:O    | 2.53                     | 0.42              |
| 22:w:28:LEU:O     | 22:w:29:ALA:C    | 2.62                     | 0.42              |
| 32:G:94:ARG:O     | 32:G:95:TRP:C    | 2.62                     | 0.42              |
| 33:H:178:ARG:HH11 | 33:H:178:ARG:CB  | 2.30                     | 0.42              |
| 34:I:72:ARG:HH11  | 34:I:72:ARG:HG3  | 1.84                     | 0.42              |
| 37:L:110:ARG:HG3  | 37:L:118:ARG:HG3 | 2.00                     | 0.42              |
| 37:L:134:VAL:O    | 37:L:137:ARG:HB3 | 2.19                     | 0.42              |
| 39:N:12:LYS:C     | 39:N:14:SER:H    | 2.27                     | 0.42              |
| 41:P:118:ASN:HB2  | 53:3:718:A:H5'   | 2.00                     | 0.42              |
| 43:R:94:LEU:O     | 43:R:95:PRO:C    | 2.61                     | 0.42              |
| 50:Y:25:SER:O     | 50:Y:28:ARG:HB3  | 2.19                     | 0.42              |
| 50:Y:85:LEU:HD23  | 50:Y:85:LEU:C    | 2.44                     | 0.42              |
| 51:Z:11:PHE:N     | 51:Z:11:PHE:CD1  | 2.88                     | 0.42              |
| 51:Z:44:ARG:NH1   | 51:Z:45:LYS:HA   | 2.33                     | 0.42              |
| 52:a:48:LEU:HA    | 52:a:209:ILE:HA  | 2.02                     | 0.42              |
| 52:a:161:VAL:HG22 | 52:a:162:ARG:N   | 2.34                     | 0.42              |
| 52:a:170:ILE:HG22 | 52:a:171:ILE:N   | 2.34                     | 0.42              |
| 53:3:234:C:O2'    | 53:3:235:C:H5'   | 2.19                     | 0.42              |
| 53:3:471:U:H2'    | 53:3:472:U:C6    | 2.54                     | 0.42              |
| 53:3:529:G:C4'    | 53:3:533:A:C2    | 3.03                     | 0.42              |
| 53:3:554:A:H2'    | 53:3:555:U:C6    | 2.55                     | 0.42              |
| 53:3:560:A:H4'    | 53:3:561:U:C5'   | 2.48                     | 0.42              |
| 53:3:675:A:H2'    | 53:3:676:A:H8    | 1.84                     | 0.42              |
| 53:3:909:A:H2'    | 53:3:910:C:O4'   | 2.18                     | 0.42              |
| 53:3:924:C:H2'    | 53:3:925:G:C8    | 2.54                     | 0.42              |
| 53:3:946:A:O2'    | 53:3:1333:A:N3   | 2.37                     | 0.42              |
| 53:3:1062:U:O2    | 53:3:1194:U:O4   | 2.38                     | 0.42              |
| 53:3:1105:A:H2'   | 53:3:1106:G:H8   | 1.84                     | 0.42              |
| 53:3:1326:U:O2'   | 53:3:1327:C:H5'  | 2.18                     | 0.42              |
| 53:3:1430:A:H2'   | 53:3:1431:A:H5'  | 2.01                     | 0.42              |
| 54:1:717:C:H2'    | 54:1:718:A:H5'   | 2.01                     | 0.42              |
| 54:1:859:G:H1'    | 54:1:860:U:H5    | 1.84                     | 0.42              |
| 54:1:863:A:O2'    | 54:1:864:G:H5'   | 2.19                     | 0.42              |
| 54:1:1447:C:H2'   | 54:1:1448:G:C8   | 2.54                     | 0.42              |
| 54:1:2055:C:H5'   | 54:1:2056:G:C5'  | 2.49                     | 0.42              |
| 54:1:2243:U:C2    | 54:1:2244:U:C5   | 3.07                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 55:2:6:G:H2'     | 55:2:7:G:H8       | 1.84                     | 0.42              |
| 57:6:62:C:H2'    | 57:6:63:G:C8      | 2.55                     | 0.42              |
| 3:d:131:THR:HG22 | 3:d:160:ALA:O     | 2.19                     | 0.42              |
| 4:e:6:TYR:CE1    | 4:e:10:GLU:HG2    | 2.54                     | 0.42              |
| 10:k:105:ARG:NH2 | 15:p:31:VAL:HG21  | 2.34                     | 0.42              |
| 11:l:64:PHE:O    | 30:E:14:LYS:NZ    | 2.53                     | 0.42              |
| 11:l:78:ARG:CB   | 11:l:78:ARG:HH21  | 2.32                     | 0.42              |
| 11:l:93:ASN:O    | 11:l:94:THR:HB    | 2.19                     | 0.42              |
| 11:l:141:LYS:NZ  | 11:l:143:GLU:HB3  | 2.34                     | 0.42              |
| 16:q:46:TYR:CZ   | 17:r:76:LYS:HE2   | 2.55                     | 0.42              |
| 20:u:96:LYS:C    | 20:u:98:ASN:H     | 2.27                     | 0.42              |
| 21:v:42:LEU:HD12 | 21:v:42:LEU:O     | 2.18                     | 0.42              |
| 25:z:41:PRO:HA   | 25:z:44:ARG:HG2   | 2.02                     | 0.42              |
| 27:B:43:THR:HG23 | 27:B:47:TYR:O     | 2.19                     | 0.42              |
| 32:G:71:THR:O    | 32:G:72:LYS:C     | 2.62                     | 0.42              |
| 33:H:57:GLU:O    | 33:H:64:ARG:N     | 2.49                     | 0.42              |
| 37:L:115:MET:HG2 | 37:L:118:ARG:HH21 | 1.84                     | 0.42              |
| 38:M:4:ASP:OD2   | 38:M:76:ARG:NH1   | 2.52                     | 0.42              |
| 40:O:7:ARG:CG    | 40:O:75:ASP:HB2   | 2.46                     | 0.42              |
| 40:O:72:ARG:HG3  | 40:O:72:ARG:HH11  | 1.83                     | 0.42              |
| 46:U:32:PHE:C    | 46:U:33:ILE:HD12  | 2.45                     | 0.42              |
| 48:W:12:PHE:O    | 48:W:13:THR:C     | 2.62                     | 0.42              |
| 49:X:39:ILE:HA   | 49:X:43:MET:HE2   | 2.01                     | 0.42              |
| 51:Z:9:GLU:CB    | 51:Z:10:PRO:CD    | 2.88                     | 0.42              |
| 52:a:33:LEU:HD21 | 52:a:222:VAL:HG23 | 2.01                     | 0.42              |
| 53:3:335:C:H2'   | 53:3:336:A:C8     | 2.54                     | 0.42              |
| 53:3:665:A:C1'   | 53:3:733:G:H1'    | 2.48                     | 0.42              |
| 53:3:1126:U:H1'  | 53:3:1281:C:C4    | 2.55                     | 0.42              |
| 53:3:1172:C:C2   | 53:3:1173:U:C5    | 3.07                     | 0.42              |
| 54:1:777:G:N7    | 54:1:793:A:H2     | 2.17                     | 0.42              |
| 54:1:969:G:H2'   | 54:1:970:U:H6     | 1.84                     | 0.42              |
| 54:1:1077:A:H2'  | 54:1:1078:U:O4'   | 2.19                     | 0.42              |
| 54:1:1405:U:H2'  | 54:1:1406:U:H6    | 1.84                     | 0.42              |
| 54:1:1405:U:O2'  | 54:1:1406:U:H5'   | 2.19                     | 0.42              |
| 54:1:1561:C:H2'  | 54:1:1562:U:C6    | 2.55                     | 0.42              |
| 54:1:1760:C:H2'  | 54:1:1761:C:O4'   | 2.18                     | 0.42              |
| 54:1:2173:A:H2'  | 54:1:2173:A:N3    | 2.35                     | 0.42              |
| 54:1:2673:G:H2'  | 54:1:2674:G:H8    | 1.85                     | 0.42              |
| 59:8:99:VAL:O    | 59:8:100:GLU:C    | 2.63                     | 0.42              |
| 59:8:146:ARG:HG2 | 59:8:147:MET:N    | 2.34                     | 0.42              |
| 1:b:261:ARG:HG2  | 1:b:261:ARG:HH11  | 1.85                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:c:13:ARG:NH1   | 54:1:2683:C:H4'   | 2.33                     | 0.42              |
| 3:d:19:PHE:HE2   | 3:d:188:MET:HE1   | 1.84                     | 0.42              |
| 3:d:163:ASN:HB2  | 54:1:322:A:OP2    | 2.20                     | 0.42              |
| 4:e:105:ILE:C    | 4:e:108:PRO:HD2   | 2.45                     | 0.42              |
| 12:m:33:LEU:HD11 | 12:m:128:THR:HB   | 2.01                     | 0.42              |
| 21:v:9:ARG:HG3   | 21:v:40:ILE:C     | 2.44                     | 0.42              |
| 25:z:29:ARG:NE   | 54:1:1183:U:H5''  | 2.34                     | 0.42              |
| 29:D:11:LYS:HE3  | 54:1:770:G:P      | 2.59                     | 0.42              |
| 32:G:102:ASN:O   | 32:G:106:VAL:HG23 | 2.19                     | 0.42              |
| 33:H:194:VAL:O   | 33:H:194:VAL:HG23 | 2.20                     | 0.42              |
| 35:J:15:ILE:HD11 | 35:J:37:VAL:HG23  | 2.01                     | 0.42              |
| 36:K:5:GLU:O     | 36:K:7:VAL:HG23   | 2.19                     | 0.42              |
| 38:M:9:MET:O     | 38:M:13:ILE:HG13  | 2.18                     | 0.42              |
| 39:N:46:VAL:HG22 | 39:N:79:ARG:HD3   | 2.01                     | 0.42              |
| 39:N:81:GLY:O    | 39:N:85:ALA:N     | 2.52                     | 0.42              |
| 39:N:119:LYS:C   | 39:N:121:ARG:H    | 2.28                     | 0.42              |
| 40:O:65:TYR:HB3  | 44:S:96:LYS:O     | 2.19                     | 0.42              |
| 42:Q:7:VAL:HG22  | 47:V:30:HIS:CD2   | 2.53                     | 0.42              |
| 43:R:94:LEU:HB3  | 43:R:95:PRO:HD2   | 2.01                     | 0.42              |
| 45:T:46:LYS:O    | 45:T:47:LYS:HD3   | 2.19                     | 0.42              |
| 47:V:17:GLU:OE1  | 47:V:17:GLU:HA    | 2.19                     | 0.42              |
| 48:W:12:PHE:CD2  | 48:W:13:THR:HG22  | 2.55                     | 0.42              |
| 50:Y:79:THR:O    | 50:Y:82:ILE:HG12  | 2.20                     | 0.42              |
| 53:3:149:A:H1'   | 53:3:1446:A:H2    | 1.85                     | 0.42              |
| 53:3:721:G:H8    | 53:3:721:G:OP1    | 2.02                     | 0.42              |
| 53:3:837:U:H2'   | 53:3:838:G:H8     | 1.83                     | 0.42              |
| 53:3:892:A:H2'   | 53:3:893:C:C6     | 2.54                     | 0.42              |
| 53:3:948:C:H2'   | 53:3:949:A:H8     | 1.85                     | 0.42              |
| 53:3:1406:U:H2'  | 53:3:1407:C:O4'   | 2.19                     | 0.42              |
| 54:1:533:G:H2'   | 54:1:534:U:O4'    | 2.20                     | 0.42              |
| 54:1:575:A:O2'   | 54:1:576:U:H5'    | 2.19                     | 0.42              |
| 54:1:1313:U:O2   | 54:1:1313:U:H2'   | 2.19                     | 0.42              |
| 54:1:1548:A:H2'  | 54:1:1549:A:H8    | 1.84                     | 0.42              |
| 54:1:1925:C:O2'  | 54:1:1926:U:H5'   | 2.20                     | 0.42              |
| 54:1:2043:C:C2   | 54:1:2044:C:C5    | 3.07                     | 0.42              |
| 54:1:2163:A:H3'  | 54:1:2164:C:C5'   | 2.50                     | 0.42              |
| 54:1:2294:G:O2'  | 54:1:2295:C:H5'   | 2.20                     | 0.42              |
| 54:1:2414:G:C6   | 54:1:2415:G:N7    | 2.87                     | 0.42              |
| 54:1:2455:G:C4   | 54:1:2456:C:C5    | 3.08                     | 0.42              |
| 54:1:2475:C:H2'  | 54:1:2476:A:H5'   | 2.01                     | 0.42              |
| 54:1:2625:G:H2'  | 54:1:2626:C:O4'   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 54:1:2650:U:H2'   | 54:1:2651:C:H6   | 1.83                     | 0.42              |
| 54:1:2802:G:H2'   | 54:1:2803:G:H8   | 1.84                     | 0.42              |
| 56:5:10:G:C2      | 56:5:26:A:H1'    | 2.54                     | 0.42              |
| 56:5:11:C:H2'     | 56:5:12:G:H8     | 1.83                     | 0.42              |
| 59:8:326:THR:HG23 | 59:8:332:ASN:HA  | 2.01                     | 0.42              |
| 59:8:561:LEU:HD23 | 59:8:561:LEU:C   | 2.44                     | 0.42              |
| 59:8:571:VAL:HG12 | 59:8:572:VAL:N   | 2.34                     | 0.42              |
| 59:8:590:GLU:HG3  | 59:8:591:LEU:N   | 2.34                     | 0.42              |
| 59:8:637:ARG:HB3  | 59:8:637:ARG:NH1 | 2.35                     | 0.42              |
| 2:c:36:GLN:HG2    | 2:c:37:VAL:N     | 2.35                     | 0.42              |
| 2:c:47:ALA:HB2    | 2:c:83:ARG:HD2   | 2.01                     | 0.42              |
| 6:g:16:GLY:HA2    | 6:g:47:PHE:CE2   | 2.54                     | 0.42              |
| 10:k:31:ARG:HG2   | 10:k:31:ARG:NH1  | 2.34                     | 0.42              |
| 12:m:78:LEU:HD23  | 12:m:79:ALA:N    | 2.34                     | 0.42              |
| 13:n:90:ARG:HD2   | 54:1:2880:C:O2'  | 2.20                     | 0.42              |
| 16:q:79:ILE:HD11  | 16:q:91:ARG:NH2  | 2.35                     | 0.42              |
| 17:r:49:ILE:HG22  | 17:r:54:VAL:HA   | 2.01                     | 0.42              |
| 17:r:72:VAL:O     | 17:r:74:ILE:HD12 | 2.19                     | 0.42              |
| 18:s:89:ALA:HB2   | 54:1:748:G:O5'   | 2.20                     | 0.42              |
| 21:v:6:ALA:HB2    | 21:v:42:LEU:HB3  | 2.01                     | 0.42              |
| 24:y:14:LEU:O     | 24:y:17:GLU:HG3  | 2.20                     | 0.42              |
| 25:z:35:VAL:HG22  | 25:z:36:GLU:N    | 2.34                     | 0.42              |
| 36:K:2:ARG:HG2    | 36:K:2:ARG:HH11  | 1.85                     | 0.42              |
| 38:M:9:MET:SD     | 38:M:9:MET:C     | 3.03                     | 0.42              |
| 38:M:13:ILE:HD12  | 38:M:74:ILE:HD13 | 2.01                     | 0.42              |
| 39:N:17:ARG:HD3   | 53:3:1147:C:O2'  | 2.20                     | 0.42              |
| 44:S:57:SER:HB3   | 53:3:1360:A:C5   | 2.53                     | 0.42              |
| 45:T:2:LEU:HD13   | 45:T:34:GLN:HA   | 2.02                     | 0.42              |
| 46:U:74:LEU:HA    | 46:U:77:GLU:HB3  | 2.00                     | 0.42              |
| 50:Y:67:HIS:C     | 50:Y:69:ASN:N    | 2.77                     | 0.42              |
| 53:3:132:C:H2'    | 53:3:133:U:C6    | 2.54                     | 0.42              |
| 53:3:440:C:H2'    | 53:3:441:A:O4'   | 2.20                     | 0.42              |
| 53:3:825:A:H2'    | 53:3:826:C:H6    | 1.84                     | 0.42              |
| 53:3:978:A:H4'    | 53:3:1224:U:O4   | 2.20                     | 0.42              |
| 54:1:157:C:H2'    | 54:1:158:U:O4'   | 2.18                     | 0.42              |
| 54:1:365:U:H2'    | 54:1:366:C:C6    | 2.54                     | 0.42              |
| 54:1:859:G:HO2'   | 54:1:860:U:H6    | 1.59                     | 0.42              |
| 54:1:1101:U:O2'   | 54:1:1102:C:H5'  | 2.19                     | 0.42              |
| 54:1:1748:C:H2'   | 54:1:1749:A:C8   | 2.55                     | 0.42              |
| 54:1:2175:C:H2'   | 54:1:2176:A:C8   | 2.54                     | 0.42              |
| 56:5:58:A:H1'     | 56:5:60:U:OP2    | 2.18                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 59:8:17:ALA:HB2   | 59:8:112:VAL:N    | 2.31                     | 0.42              |
| 59:8:33:TYR:OH    | 59:8:199:GLY:HA3  | 2.20                     | 0.42              |
| 59:8:188:MET:HE1  | 59:8:216:ASN:HA   | 2.00                     | 0.42              |
| 59:8:243:LEU:HD22 | 59:8:247:GLU:OE1  | 2.18                     | 0.42              |
| 59:8:348:THR:HA   | 59:8:358:GLU:O    | 2.19                     | 0.42              |
| 59:8:349:VAL:HG11 | 59:8:360:PHE:CE2  | 2.53                     | 0.42              |
| 1:b:14:HIS:O      | 1:b:16:VAL:HG23   | 2.20                     | 0.42              |
| 2:c:100:LEU:HD12  | 2:c:100:LEU:N     | 2.34                     | 0.42              |
| 3:d:8:ALA:O       | 3:d:9:GLN:HB2     | 2.19                     | 0.42              |
| 5:f:34:ARG:HG2    | 5:f:35:THR:O      | 2.20                     | 0.42              |
| 6:g:37:VAL:HG21   | 6:g:51:ARG:HH12   | 1.85                     | 0.42              |
| 15:p:30:TRP:HA    | 15:p:30:TRP:HE3   | 1.84                     | 0.42              |
| 16:q:109:VAL:O    | 16:q:113:LYS:HG3  | 2.19                     | 0.42              |
| 17:r:49:ILE:HG21  | 17:r:52:PRO:HA    | 2.01                     | 0.42              |
| 20:u:66:VAL:C     | 20:u:68:ASN:H     | 2.27                     | 0.42              |
| 21:v:30:ILE:HB    | 21:v:38:LEU:HB3   | 2.02                     | 0.42              |
| 23:x:28:PHE:CD1   | 54:1:396:G:H1'    | 2.52                     | 0.42              |
| 24:y:37:LEU:HD21  | 24:y:40:SER:HA    | 2.00                     | 0.42              |
| 29:D:8:SER:HB3    | 29:D:11:LYS:HB2   | 2.00                     | 0.42              |
| 34:I:8:LEU:CB     | 53:3:430:A:OP1    | 2.67                     | 0.42              |
| 35:J:68:ARG:HB3   | 35:J:68:ARG:HH11  | 1.84                     | 0.42              |
| 36:K:44:ARG:HB2   | 36:K:58:HIS:ND1   | 2.35                     | 0.42              |
| 40:O:41:PRO:HD2   | 53:3:1150:A:N3    | 2.34                     | 0.42              |
| 40:O:73:LEU:O     | 40:O:73:LEU:HD13  | 2.20                     | 0.42              |
| 46:U:22:ALA:CB    | 46:U:32:PHE:HA    | 2.50                     | 0.42              |
| 52:a:40:GLU:O     | 52:a:178:VAL:HG13 | 2.20                     | 0.42              |
| 53:3:664:G:H22    | 53:3:741:G:H1     | 1.67                     | 0.42              |
| 53:3:1360:A:C2'   | 53:3:1361:G:H5'   | 2.50                     | 0.42              |
| 53:3:1481:U:H2'   | 53:3:1482:G:C8    | 2.54                     | 0.42              |
| 54:1:190:A:C6     | 54:1:191:A:C6     | 3.07                     | 0.42              |
| 54:1:352:A:H2'    | 54:1:353:C:C6     | 2.55                     | 0.42              |
| 54:1:493:G:H2'    | 54:1:494:G:O4'    | 2.19                     | 0.42              |
| 54:1:765:C:H2'    | 54:1:766:U:H6     | 1.85                     | 0.42              |
| 54:1:1409:U:H2'   | 54:1:1410:G:H8    | 1.85                     | 0.42              |
| 54:1:1425:G:H2'   | 54:1:1426:G:C8    | 2.55                     | 0.42              |
| 54:1:1827:U:H6    | 54:1:1827:U:O5'   | 2.02                     | 0.42              |
| 54:1:1863:G:H2'   | 54:1:1864:U:O4'   | 2.19                     | 0.42              |
| 54:1:2128:G:H1'   | 54:1:2173:A:N3    | 2.35                     | 0.42              |
| 54:1:2746:U:O4    | 54:1:2755:C:H4'   | 2.20                     | 0.42              |
| 59:8:73:SER:HA    | 59:8:80:GLU:HG3   | 2.01                     | 0.42              |
| 59:8:97:ILE:HD13  | 59:8:412:PRO:HG2  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 59:8:138:ILE:HB  | 59:8:263:LEU:HB2  | 2.00                     | 0.42              |
| 1:b:54:GLY:HA3   | 1:b:216:ARG:HD2   | 2.01                     | 0.42              |
| 2:c:46:ARG:HG2   | 2:c:46:ARG:HH11   | 1.85                     | 0.42              |
| 8:i:38:CYS:O     | 8:i:42:ASN:ND2    | 2.48                     | 0.42              |
| 11:l:70:LYS:O    | 11:l:72:ALA:N     | 2.53                     | 0.42              |
| 13:n:100:CYS:HA  | 27:B:42:ILE:HG12  | 2.01                     | 0.42              |
| 15:p:52:ARG:HB2  | 15:p:55:HIS:HB2   | 2.02                     | 0.42              |
| 17:r:60:LYS:HG2  | 17:r:100:GLY:HA3  | 2.02                     | 0.42              |
| 19:t:66:LYS:HB2  | 19:t:77:ARG:HD3   | 2.02                     | 0.42              |
| 20:u:73:ASN:HD22 | 20:u:76:THR:H     | 1.67                     | 0.42              |
| 26:A:16:CYS:SG   | 26:A:20:ASN:HB2   | 2.60                     | 0.42              |
| 26:A:61:ASN:HA   | 26:A:64:PHE:HB2   | 2.00                     | 0.42              |
| 28:C:4:ILE:O     | 28:C:4:ILE:HG22   | 2.19                     | 0.42              |
| 29:D:13:ASN:O    | 29:D:17:GLY:HA3   | 2.20                     | 0.42              |
| 32:G:71:THR:O    | 32:G:76:SER:HB3   | 2.20                     | 0.42              |
| 33:H:22:PHE:HD2  | 40:O:97:ASP:OD1   | 2.03                     | 0.42              |
| 34:I:100:VAL:O   | 34:I:104:MET:N    | 2.38                     | 0.42              |
| 35:J:47:PHE:HZ   | 35:J:137:ARG:HH11 | 1.66                     | 0.42              |
| 35:J:75:LEU:HD12 | 35:J:75:LEU:C     | 2.45                     | 0.42              |
| 36:K:8:PHE:HD2   | 36:K:84:VAL:HG13  | 1.85                     | 0.42              |
| 38:M:107:LYS:HG2 | 38:M:120:LEU:HD13 | 2.01                     | 0.42              |
| 41:P:35:ASP:OD1  | 41:P:39:ASN:HB2   | 2.19                     | 0.42              |
| 42:Q:57:THR:OG1  | 53:3:362:G:OP1    | 2.36                     | 0.42              |
| 44:S:40:ARG:HD3  | 49:X:6:LYS:HZ2    | 1.84                     | 0.42              |
| 47:V:16:MET:HE2  | 53:3:254:G:O4'    | 2.19                     | 0.42              |
| 51:Z:6:ARG:C     | 51:Z:8:ASN:N      | 2.74                     | 0.42              |
| 51:Z:64:ALA:C    | 51:Z:66:ARG:H     | 2.28                     | 0.42              |
| 53:3:63:C:H4'    | 53:3:380:G:C4'    | 2.49                     | 0.42              |
| 53:3:222:C:H2'   | 53:3:223:A:C8     | 2.55                     | 0.42              |
| 53:3:280:C:O2'   | 53:3:281:G:P      | 2.77                     | 0.42              |
| 53:3:710:G:H2'   | 53:3:711:G:O4'    | 2.20                     | 0.42              |
| 53:3:908:A:O2'   | 53:3:909:A:H5'    | 2.20                     | 0.42              |
| 53:3:1188:A:H2'  | 53:3:1189:U:O4'   | 2.20                     | 0.42              |
| 53:3:1324:A:O4'  | 53:3:1362:A:H4'   | 2.20                     | 0.42              |
| 54:1:236:C:H2'   | 54:1:237:C:H6     | 1.85                     | 0.42              |
| 54:1:799:G:H3'   | 54:1:800:A:C8     | 2.52                     | 0.42              |
| 54:1:1509:A:H2'  | 54:1:1510:G:H8    | 1.76                     | 0.42              |
| 54:1:1909:C:H2'  | 54:1:1910:G:C8    | 2.55                     | 0.42              |
| 54:1:2290:G:H2'  | 54:1:2291:U:C6    | 2.55                     | 0.42              |
| 54:1:2710:C:H2'  | 54:1:2711:A:H8    | 1.83                     | 0.42              |
| 54:1:2785:C:H2'  | 54:1:2786:U:H6    | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 56:5:23:C:H2'     | 56:5:24:G:C8      | 2.54                     | 0.42              |
| 59:8:338:VAL:N    | 59:8:381:ASP:O    | 2.49                     | 0.42              |
| 59:8:553:VAL:CG1  | 59:8:593:PHE:HB3  | 2.49                     | 0.42              |
| 59:8:599:ILE:HD12 | 59:8:599:ILE:H    | 1.83                     | 0.42              |
| 1:b:44:ASN:OD1    | 1:b:45:ASN:ND2    | 2.53                     | 0.42              |
| 1:b:94:LEU:HB3    | 1:b:100:ARG:HG2   | 2.02                     | 0.42              |
| 1:b:211:ARG:HG2   | 1:b:211:ARG:NH1   | 2.34                     | 0.42              |
| 1:b:257:ARG:HD2   | 1:b:269:ARG:HH12  | 1.83                     | 0.42              |
| 2:c:122:VAL:HG21  | 2:c:141:ARG:HB3   | 2.02                     | 0.42              |
| 2:c:148:GLN:CD    | 2:c:148:GLN:N     | 2.78                     | 0.42              |
| 3:d:12:LEU:HD23   | 3:d:13:THR:O      | 2.19                     | 0.42              |
| 5:f:37:ASN:HB3    | 5:f:40:VAL:HG23   | 2.02                     | 0.42              |
| 9:j:100:VAL:HB    | 9:j:101:ILE:HD12  | 2.02                     | 0.42              |
| 9:j:111:LYS:HD2   | 9:j:111:LYS:N     | 2.34                     | 0.42              |
| 16:q:56:PHE:HB3   | 16:q:60:TRP:CZ2   | 2.55                     | 0.42              |
| 27:B:32:THR:HB    | 27:B:50:GLY:HA2   | 2.01                     | 0.42              |
| 32:G:66:ILE:HB    | 32:G:88:GLN:HG3   | 2.02                     | 0.42              |
| 33:H:3:LYS:HA     | 53:3:1190:G:H5''  | 2.01                     | 0.42              |
| 33:H:180:ASP:OD2  | 33:H:206:ILE:N    | 2.52                     | 0.42              |
| 35:J:153:ALA:HA   | 35:J:163:ILE:HD13 | 2.02                     | 0.42              |
| 36:K:90:MET:HE1   | 53:3:736:C:H5''   | 2.01                     | 0.42              |
| 37:L:35:LYS:O     | 37:L:39:GLU:HG3   | 2.20                     | 0.42              |
| 38:M:55:LYS:HE3   | 53:3:653:U:O2     | 2.19                     | 0.42              |
| 39:N:4:GLN:HA     | 39:N:20:ILE:O     | 2.19                     | 0.42              |
| 39:N:79:ARG:HD2   | 39:N:102:PHE:CE1  | 2.55                     | 0.42              |
| 44:S:52:ARG:HG3   | 53:3:1317:C:N3    | 2.34                     | 0.42              |
| 44:S:91:GLU:O     | 44:S:93:PRO:HD3   | 2.19                     | 0.42              |
| 47:V:20:ILE:HG22  | 47:V:45:VAL:O     | 2.20                     | 0.42              |
| 50:Y:28:ARG:O     | 50:Y:32:LYS:HG2   | 2.19                     | 0.42              |
| 51:Z:35:GLU:O     | 51:Z:36:PHE:HB2   | 2.19                     | 0.42              |
| 53:3:518:C:H5'    | 53:3:530:G:C4'    | 2.49                     | 0.42              |
| 53:3:548:G:H2'    | 53:3:549:C:C6     | 2.55                     | 0.42              |
| 53:3:1424:U:H2'   | 53:3:1425:U:C6    | 2.54                     | 0.42              |
| 54:1:122:G:O2'    | 54:1:123:G:H5'    | 2.20                     | 0.42              |
| 54:1:444:C:O2'    | 54:1:445:C:H5'    | 2.20                     | 0.42              |
| 54:1:766:U:H2'    | 54:1:767:U:C6     | 2.55                     | 0.42              |
| 54:1:827:U:H4'    | 54:1:828:U:C5     | 2.54                     | 0.42              |
| 54:1:1251:C:O2'   | 54:1:1252:G:H3'   | 2.19                     | 0.42              |
| 54:1:1287:A:O2'   | 54:1:1288:G:H5'   | 2.19                     | 0.42              |
| 54:1:1766:G:O2'   | 54:1:1767:G:H5'   | 2.20                     | 0.42              |
| 54:1:2112:G:H21   | 57:6:19:G:H1      | 1.67                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 54:1:2179:C:H2'  | 54:1:2180:U:C5    | 2.54                     | 0.42              |
| 54:1:2360:G:H2'  | 54:1:2361:G:H5'   | 2.02                     | 0.42              |
| 54:1:2785:C:O2'  | 54:1:2786:U:H5'   | 2.20                     | 0.42              |
| 59:8:159:LYS:HG2 | 59:8:166:PRO:CD   | 2.50                     | 0.42              |
| 2:c:129:THR:HG22 | 2:c:130:GLN:N     | 2.34                     | 0.42              |
| 4:e:39:VAL:O     | 4:e:41:GLU:HG2    | 2.20                     | 0.42              |
| 4:e:100:GLU:HG3  | 4:e:101:ARG:N     | 2.35                     | 0.42              |
| 4:e:150:GLY:O    | 54:1:2305:U:N3    | 2.53                     | 0.42              |
| 20:u:31:GLY:C    | 20:u:66:VAL:HG23  | 2.44                     | 0.42              |
| 22:w:70:PRO:HD3  | 55:2:12:C:N4      | 2.35                     | 0.42              |
| 26:A:11:GLU:HG2  | 26:A:23:LYS:HZ3   | 1.84                     | 0.42              |
| 29:D:34:ARG:CZ   | 29:D:39:ARG:HD2   | 2.50                     | 0.42              |
| 33:H:80:GLY:HA2  | 33:H:83:VAL:CG2   | 2.49                     | 0.42              |
| 38:M:90:GLU:O    | 38:M:90:GLU:HG2   | 2.20                     | 0.42              |
| 41:P:12:ARG:HG2  | 41:P:75:GLU:OE1   | 2.20                     | 0.42              |
| 44:S:5:MET:SD    | 53:3:982:U:H5''   | 2.60                     | 0.42              |
| 47:V:39:ARG:HA   | 47:V:39:ARG:HD2   | 1.88                     | 0.42              |
| 48:W:42:ARG:HG3  | 48:W:43:ILE:N     | 2.35                     | 0.42              |
| 49:X:2:ARG:N     | 53:3:1312:G:C6    | 2.88                     | 0.42              |
| 50:Y:2:ASN:O     | 50:Y:7:LYS:HE2    | 2.20                     | 0.42              |
| 53:3:181:A:N6    | 53:3:194:C:H2'    | 2.35                     | 0.42              |
| 53:3:184:G:H4'   | 53:3:224:U:H4'    | 2.02                     | 0.42              |
| 53:3:211:G:H2'   | 53:3:212:G:C4'    | 2.50                     | 0.42              |
| 53:3:372:C:N4    | 53:3:387:U:H2'    | 2.35                     | 0.42              |
| 53:3:556:C:O2'   | 53:3:557:G:H5'    | 2.19                     | 0.42              |
| 53:3:596:A:H5'   | 53:3:596:A:C8     | 2.54                     | 0.42              |
| 53:3:756:C:O2'   | 53:3:757:U:H5'    | 2.19                     | 0.42              |
| 53:3:1026:G:H21  | 53:3:1027:C:H1'   | 1.85                     | 0.42              |
| 53:3:1122:U:O4   | 53:3:1150:A:N6    | 2.53                     | 0.42              |
| 53:3:1289:A:H2'  | 53:3:1290:G:H5'   | 2.01                     | 0.42              |
| 54:1:28:A:O2'    | 54:1:29:U:H5'     | 2.20                     | 0.42              |
| 54:1:571:U:C4    | 54:1:2030:A:C6    | 3.08                     | 0.42              |
| 54:1:738:G:O2'   | 54:1:739:A:H5'    | 2.20                     | 0.42              |
| 54:1:1665:A:H2'  | 54:1:1666:G:O4'   | 2.19                     | 0.42              |
| 54:1:2398:U:H2'  | 54:1:2399:G:H8    | 1.83                     | 0.42              |
| 54:1:2811:G:H2'  | 54:1:2812:G:H8    | 1.85                     | 0.42              |
| 54:1:2826:A:H2'  | 54:1:2827:C:H6    | 1.84                     | 0.42              |
| 54:1:2830:C:O2'  | 54:1:2831:G:H5'   | 2.20                     | 0.42              |
| 59:8:187:LYS:HB2 | 59:8:189:LYS:HG2  | 2.01                     | 0.42              |
| 59:8:244:THR:O   | 59:8:248:ILE:HG12 | 2.19                     | 0.42              |
| 1:b:106:PRO:CG   | 1:b:109:LEU:HD22  | 2.50                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:b:252:LYS:HD3   | 54:1:1901:A:H4'  | 2.02                     | 0.42              |
| 3:d:76:PRO:HA     | 3:d:81:GLY:O     | 2.20                     | 0.42              |
| 3:d:126:VAL:HG22  | 3:d:127:GLU:N    | 2.35                     | 0.42              |
| 6:g:1:MET:HG3     | 6:g:3:VAL:CG2    | 2.49                     | 0.42              |
| 8:i:3:LYS:HE3     | 8:i:3:LYS:HB3    | 1.95                     | 0.42              |
| 10:k:30:ARG:CG    | 54:1:2674:G:H4'  | 2.48                     | 0.42              |
| 11:l:95:LEU:HB3   | 11:l:100:ILE:CG1 | 2.49                     | 0.42              |
| 15:p:49:ILE:HD12  | 15:p:49:ILE:N    | 2.35                     | 0.42              |
| 18:s:66:ILE:CA    | 18:s:69:LEU:HD13 | 2.45                     | 0.42              |
| 18:s:92:ARG:HH11  | 18:s:92:ARG:HG2  | 1.85                     | 0.42              |
| 23:x:40:GLU:OE1   | 23:x:63:ILE:HG21 | 2.19                     | 0.42              |
| 24:y:2:LYS:HB2    | 54:1:78:U:P      | 2.60                     | 0.42              |
| 31:F:32:LYS:CE    | 54:1:2478:A:H5'  | 2.48                     | 0.42              |
| 32:G:163:ILE:HG23 | 32:G:164:ASP:N   | 2.35                     | 0.42              |
| 33:H:71:ARG:HG2   | 33:H:71:ARG:HH11 | 1.85                     | 0.42              |
| 34:I:124:VAL:C    | 34:I:126:GLY:H   | 2.28                     | 0.42              |
| 35:J:111:ARG:HG3  | 35:J:111:ARG:NH1 | 2.32                     | 0.42              |
| 37:L:79:VAL:HG11  | 58:4:12:A:H61    | 1.85                     | 0.42              |
| 40:O:102:LEU:HD12 | 40:O:102:LEU:N   | 2.34                     | 0.42              |
| 42:Q:58:ASN:OD1   | 42:Q:60:PHE:HB2  | 2.19                     | 0.42              |
| 44:S:73:LEU:O     | 44:S:77:GLY:N    | 2.51                     | 0.42              |
| 46:U:36:VAL:O     | 46:U:36:VAL:HG13 | 2.19                     | 0.42              |
| 49:X:46:LEU:HD12  | 49:X:46:LEU:N    | 2.34                     | 0.42              |
| 53:3:280:C:HO2'   | 53:3:281:G:P     | 2.41                     | 0.42              |
| 53:3:287:U:O2'    | 53:3:288:A:H5'   | 2.20                     | 0.42              |
| 53:3:470:C:H2'    | 53:3:471:U:C6    | 2.55                     | 0.42              |
| 53:3:623:C:H2'    | 53:3:624:C:H6    | 1.83                     | 0.42              |
| 53:3:1126:U:H4'   | 53:3:1281:C:H1'  | 2.01                     | 0.42              |
| 53:3:1277:C:H4'   | 53:3:1281:C:N4   | 2.35                     | 0.42              |
| 53:3:1521:C:H2'   | 53:3:1522:U:C6   | 2.54                     | 0.42              |
| 54:1:56:A:H2'     | 54:1:57:C:O4'    | 2.19                     | 0.42              |
| 54:1:84:A:H4'     | 54:1:85:G:O5'    | 2.19                     | 0.42              |
| 54:1:162:U:C2'    | 54:1:163:C:H5'   | 2.50                     | 0.42              |
| 54:1:1218:G:H2'   | 54:1:1219:U:C6   | 2.55                     | 0.42              |
| 54:1:1429:G:O4'   | 54:1:1568:G:H1'  | 2.20                     | 0.42              |
| 54:1:1590:A:H2'   | 54:1:1591:A:C8   | 2.55                     | 0.42              |
| 54:1:1797:G:C6    | 54:1:1798:U:C4   | 3.08                     | 0.42              |
| 54:1:1922:G:H2'   | 54:1:1923:U:H6   | 1.85                     | 0.42              |
| 54:1:2039:U:H2'   | 54:1:2040:G:C8   | 2.54                     | 0.42              |
| 54:1:2171:A:H5'   | 54:1:2174:C:N4   | 2.34                     | 0.42              |
| 54:1:2183:A:H2'   | 54:1:2184:A:H8   | 1.79                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:2462:C:H1'   | 54:1:2491:U:O4    | 2.20                     | 0.42              |
| 54:1:2508:G:H2'   | 54:1:2509:G:H8    | 1.85                     | 0.42              |
| 54:1:2739:U:O2'   | 54:1:2740:A:H5'   | 2.20                     | 0.42              |
| 54:1:2834:G:H1'   | 54:1:2883:A:N6    | 2.35                     | 0.42              |
| 55:2:119:A:N3     | 55:2:120:A:N9     | 2.68                     | 0.42              |
| 59:8:473:MET:O    | 59:8:478:ASN:N    | 2.53                     | 0.42              |
| 59:8:628:THR:CG2  | 59:8:652:VAL:HG21 | 2.50                     | 0.42              |
| 8:i:18:ASN:H      | 8:i:38:CYS:CB     | 2.32                     | 0.41              |
| 9:j:55:ILE:HD11   | 9:j:130:HIS:HB2   | 2.01                     | 0.41              |
| 10:k:40:LYS:HD2   | 10:k:57:VAL:HG12  | 2.01                     | 0.41              |
| 13:n:28:LEU:CD2   | 13:n:48:VAL:HG21  | 2.50                     | 0.41              |
| 14:o:34:HIS:ND1   | 14:o:54:VAL:HA    | 2.34                     | 0.41              |
| 16:q:1:ALA:HB3    | 54:1:1248:G:OP1   | 2.20                     | 0.41              |
| 32:G:42:LEU:O     | 32:G:46:VAL:HG23  | 2.19                     | 0.41              |
| 34:I:10:LEU:HD12  | 34:I:20:LEU:CD2   | 2.50                     | 0.41              |
| 35:J:96:GLN:HE21  | 35:J:123:LEU:HD11 | 1.84                     | 0.41              |
| 37:L:109:LYS:C    | 37:L:110:ARG:HG2  | 2.44                     | 0.41              |
| 38:M:88:LYS:O     | 38:M:91:LEU:HG    | 2.20                     | 0.41              |
| 39:N:45:MET:O     | 39:N:48:ARG:N     | 2.52                     | 0.41              |
| 40:O:40:ILE:HG21  | 53:3:1124:G:C2    | 2.55                     | 0.41              |
| 42:Q:49:ARG:HD2   | 42:Q:89:LEU:CD1   | 2.50                     | 0.41              |
| 42:Q:56:LEU:HD11  | 42:Q:62:VAL:HG22  | 2.02                     | 0.41              |
| 43:R:18:LEU:HD21  | 43:R:32:ILE:HG13  | 2.01                     | 0.41              |
| 45:T:36:ASN:O     | 45:T:39:GLN:HB3   | 2.20                     | 0.41              |
| 48:W:40:PRO:HG2   | 48:W:43:ILE:CG1   | 2.49                     | 0.41              |
| 53:3:635:A:H2'    | 53:3:636:U:H6     | 1.85                     | 0.41              |
| 53:3:850:U:C3'    | 53:3:851:G:H5''   | 2.49                     | 0.41              |
| 53:3:967:C:C5     | 53:3:968:A:C6     | 3.08                     | 0.41              |
| 53:3:1432:G:H1'   | 53:3:1468:A:H62   | 1.84                     | 0.41              |
| 54:1:302:C:H2'    | 54:1:303:G:H8     | 1.85                     | 0.41              |
| 54:1:568:U:H2'    | 54:1:570:G:OP2    | 2.20                     | 0.41              |
| 54:1:1565:C:O2'   | 54:1:1566:A:C8    | 2.73                     | 0.41              |
| 54:1:1930:G:O2'   | 54:1:1931:U:C6    | 2.72                     | 0.41              |
| 54:1:1998:A:O2'   | 54:1:1999:C:H5'   | 2.20                     | 0.41              |
| 54:1:2832:U:H1'   | 54:1:2834:G:C4    | 2.54                     | 0.41              |
| 59:8:491:ARG:CD   | 59:8:570:PRO:HB2  | 2.50                     | 0.41              |
| 59:8:519:VAL:HG21 | 59:8:580:PHE:HB3  | 2.01                     | 0.41              |
| 1:b:129:LEU:CD1   | 1:b:134:ILE:HG12  | 2.50                     | 0.41              |
| 1:b:211:ARG:HH12  | 54:1:781:A:N6     | 2.18                     | 0.41              |
| 3:d:40:ARG:HG2    | 3:d:40:ARG:NH1    | 2.32                     | 0.41              |
| 3:d:143:LEU:HD22  | 3:d:185:LYS:HG3   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:g:9:VAL:C       | 6:g:11:ASN:H      | 2.27                     | 0.41              |
| 8:i:36:GLU:HB3    | 8:i:66:PHE:HZ     | 1.85                     | 0.41              |
| 9:j:37:ARG:HG3    | 9:j:37:ARG:HH21   | 1.84                     | 0.41              |
| 10:k:1:MET:HE3    | 54:l:1664:A:H2    | 1.85                     | 0.41              |
| 12:m:78:LEU:HD23  | 12:m:79:ALA:CB    | 2.50                     | 0.41              |
| 17:r:39:LEU:HD12  | 17:r:39:LEU:N     | 2.34                     | 0.41              |
| 32:G:94:ARG:HH22  | 32:G:145:ASN:HD21 | 1.68                     | 0.41              |
| 33:H:130:ARG:HA   | 33:H:133:MET:HE2  | 2.01                     | 0.41              |
| 34:I:58:GLN:O     | 34:I:62:ARG:HG2   | 2.21                     | 0.41              |
| 34:I:115:GLN:HE22 | 34:I:153:ARG:HH12 | 1.68                     | 0.41              |
| 40:O:88:MET:O     | 40:O:90:LEU:N     | 2.53                     | 0.41              |
| 42:Q:29:LYS:HZ2   | 42:Q:57:THR:CG2   | 2.33                     | 0.41              |
| 43:R:100:ARG:HG2  | 43:R:100:ARG:NH1  | 2.35                     | 0.41              |
| 49:X:47:THR:HA    | 49:X:59:VAL:O     | 2.20                     | 0.41              |
| 50:Y:63:LYS:NZ    | 53:3:177:G:OP2    | 2.49                     | 0.41              |
| 51:Z:23:GLU:CG    | 51:Z:24:LYS:H     | 2.32                     | 0.41              |
| 53:3:821:G:H2'    | 53:3:822:U:C6     | 2.55                     | 0.41              |
| 53:3:1059:C:H2'   | 53:3:1060:U:O4'   | 2.20                     | 0.41              |
| 53:3:1347:G:H22   | 53:3:1374:A:P     | 2.42                     | 0.41              |
| 53:3:1507:A:H2'   | 53:3:1508:A:H8    | 1.83                     | 0.41              |
| 54:1:52:A:O2'     | 54:1:53:A:H5'     | 2.20                     | 0.41              |
| 54:1:175:G:O2'    | 54:1:176:A:H5'    | 2.21                     | 0.41              |
| 54:1:1023:U:O2'   | 54:1:1122:G:H5'   | 2.20                     | 0.41              |
| 54:1:1061:U:H2'   | 54:1:1062:G:H5''  | 2.01                     | 0.41              |
| 54:1:1357:C:H2'   | 54:1:1358:G:O4'   | 2.20                     | 0.41              |
| 54:1:2316:G:O2'   | 54:1:2317:A:H5'   | 2.20                     | 0.41              |
| 54:1:2340:A:H2'   | 54:1:2341:G:H8    | 1.85                     | 0.41              |
| 54:1:2447:G:C8    | 54:1:2501:C:C6    | 3.09                     | 0.41              |
| 55:2:97:C:C2'     | 55:2:98:G:H5'     | 2.50                     | 0.41              |
| 55:2:118:C:N3     | 55:2:119:A:N7     | 2.68                     | 0.41              |
| 56:5:27:A:H2'     | 56:5:28:C:C6      | 2.55                     | 0.41              |
| 59:8:13:ILE:O     | 59:8:86:ILE:HD12  | 2.20                     | 0.41              |
| 59:8:183:VAL:O    | 59:8:183:VAL:HG13 | 2.20                     | 0.41              |
| 59:8:694:VAL:HA   | 59:8:697:ALA:HB3  | 2.00                     | 0.41              |
| 5:f:23:ILE:HG22   | 5:f:24:THR:N      | 2.36                     | 0.41              |
| 9:j:2:LYS:HE2     | 9:j:2:LYS:CA      | 2.50                     | 0.41              |
| 10:k:92:GLU:O     | 10:k:93:GLN:C     | 2.63                     | 0.41              |
| 10:k:110:GLU:HA   | 10:k:113:MET:HE3  | 2.02                     | 0.41              |
| 12:m:53:MET:CE    | 12:m:105:MET:HE2  | 2.50                     | 0.41              |
| 12:m:78:LEU:HD23  | 12:m:78:LEU:C     | 2.45                     | 0.41              |
| 15:p:52:ARG:HG3   | 15:p:52:ARG:HH11  | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:w:16:ARG:N     | 22:w:16:ARG:HD2   | 2.36                     | 0.41              |
| 24:y:8:GLU:HB3    | 24:y:12:GLU:OE2   | 2.21                     | 0.41              |
| 25:z:25:GLY:C     | 25:z:46:MET:HE1   | 2.45                     | 0.41              |
| 32:G:42:LEU:N     | 32:G:42:LEU:HD22  | 2.35                     | 0.41              |
| 32:G:56:LEU:HD23  | 32:G:59:ILE:HD11  | 2.02                     | 0.41              |
| 34:I:50:TYR:CD2   | 53:3:509:A:H5'    | 2.46                     | 0.41              |
| 36:K:6:ILE:HA     | 36:K:89:VAL:HA    | 2.01                     | 0.41              |
| 39:N:22:PRO:HA    | 39:N:60:LEU:HA    | 2.03                     | 0.41              |
| 39:N:112:ARG:HD3  | 44:S:100:TRP:NE1  | 2.35                     | 0.41              |
| 40:O:92:LEU:O     | 40:O:93:ALA:HB3   | 2.21                     | 0.41              |
| 42:Q:30:ARG:CD    | 42:Q:101:LEU:HD21 | 2.50                     | 0.41              |
| 43:R:33:LEU:CD2   | 43:R:40:GLU:HA    | 2.51                     | 0.41              |
| 43:R:97:ARG:O     | 53:3:1307:U:C5    | 2.73                     | 0.41              |
| 50:Y:38:ILE:CD1   | 50:Y:81:GLN:HB3   | 2.47                     | 0.41              |
| 52:a:21:TYR:N     | 52:a:223:ALA:O    | 2.53                     | 0.41              |
| 52:a:45:ALA:HA    | 52:a:171:ILE:O    | 2.19                     | 0.41              |
| 52:a:57:GLN:O     | 52:a:201:PRO:HG2  | 2.20                     | 0.41              |
| 52:a:214:ILE:HG12 | 52:a:222:VAL:O    | 2.20                     | 0.41              |
| 52:a:216:THR:OG1  | 52:a:219:GLY:HA3  | 2.20                     | 0.41              |
| 53:3:448:A:H3'    | 53:3:449:G:C8     | 2.55                     | 0.41              |
| 53:3:687:A:N6     | 53:3:703:G:O2'    | 2.53                     | 0.41              |
| 53:3:721:G:H4'    | 53:3:722:G:O4'    | 2.20                     | 0.41              |
| 53:3:1233:G:C6    | 53:3:1234:C:C4    | 3.07                     | 0.41              |
| 54:1:279:A:H2'    | 54:1:280:U:C5'    | 2.50                     | 0.41              |
| 54:1:467:G:O2'    | 54:1:468:G:H5'    | 2.20                     | 0.41              |
| 54:1:481:G:O2'    | 54:1:506:G:N2     | 2.53                     | 0.41              |
| 54:1:615:U:H5''   | 54:1:616:A:OP2    | 2.21                     | 0.41              |
| 54:1:1001:A:H2'   | 54:1:1002:G:H5'   | 2.01                     | 0.41              |
| 54:1:1006:C:O2'   | 54:1:1007:C:H5'   | 2.20                     | 0.41              |
| 55:2:1:U:C4       | 55:2:2:G:N7       | 2.88                     | 0.41              |
| 59:8:26:THR:O     | 59:8:30:ILE:HG12  | 2.19                     | 0.41              |
| 59:8:365:GLN:O    | 59:8:372:GLU:HB3  | 2.20                     | 0.41              |
| 59:8:460:GLY:HA3  | 59:8:466:LEU:HD11 | 2.01                     | 0.41              |
| 4:e:11:VAL:O      | 4:e:15:LEU:HD23   | 2.20                     | 0.41              |
| 4:e:147:ARG:HB3   | 4:e:149:ARG:HD2   | 2.01                     | 0.41              |
| 6:g:4:ILE:O       | 6:g:36:ALA:HB1    | 2.20                     | 0.41              |
| 7:h:44:ALA:O      | 7:h:47:GLU:HB3    | 2.20                     | 0.41              |
| 9:j:88:THR:CG2    | 9:j:91:GLU:HG3    | 2.50                     | 0.41              |
| 11:l:70:LYS:HE2   | 54:1:2405:G:OP1   | 2.20                     | 0.41              |
| 12:m:30:SER:HA    | 12:m:133:LYS:HB2  | 2.03                     | 0.41              |
| 13:n:74:GLU:O     | 13:n:77:ALA:HB3   | 2.19                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 16:q:116:LEU:HD23 | 16:q:116:LEU:C   | 2.45                     | 0.41              |
| 17:r:7:SER:OG     | 17:r:22:LEU:HD22 | 2.20                     | 0.41              |
| 33:H:71:ARG:HG2   | 33:H:71:ARG:NH1  | 2.35                     | 0.41              |
| 33:H:86:LEU:O     | 33:H:90:VAL:HG23 | 2.20                     | 0.41              |
| 36:K:86:ARG:NH1   | 36:K:86:ARG:HB2  | 2.36                     | 0.41              |
| 39:N:26:LYS:O     | 39:N:61:ASP:HB2  | 2.21                     | 0.41              |
| 40:O:65:TYR:HD1   | 44:S:97:LYS:HA   | 1.85                     | 0.41              |
| 41:P:53:GLY:HA2   | 41:P:56:LYS:HE3  | 2.02                     | 0.41              |
| 42:Q:29:LYS:O     | 42:Q:80:LEU:HD12 | 2.21                     | 0.41              |
| 42:Q:106:VAL:HB   | 42:Q:109:ARG:HG3 | 2.03                     | 0.41              |
| 42:Q:110:LYS:HG3  | 53:3:538:G:O3'   | 2.20                     | 0.41              |
| 43:R:52:ILE:O     | 43:R:55:LEU:HB2  | 2.20                     | 0.41              |
| 43:R:96:VAL:O     | 43:R:97:ARG:NE   | 2.53                     | 0.41              |
| 44:S:2:LYS:NZ     | 53:3:1049:U:C2   | 2.70                     | 0.41              |
| 48:W:54:LEU:HA    | 48:W:57:ALA:HB3  | 2.02                     | 0.41              |
| 52:a:5:THR:O      | 52:a:9:ARG:HB2   | 2.20                     | 0.41              |
| 53:3:90:C:H2'     | 53:3:91:U:C5     | 2.55                     | 0.41              |
| 53:3:946:A:N6     | 53:3:1236:A:C6   | 2.88                     | 0.41              |
| 54:1:225:C:H2'    | 54:1:226:A:O4'   | 2.19                     | 0.41              |
| 54:1:441:U:H2'    | 54:1:442:G:H8    | 1.83                     | 0.41              |
| 54:1:524:G:O2'    | 54:1:525:U:H5'   | 2.20                     | 0.41              |
| 54:1:588:U:O4     | 54:1:670:A:H1'   | 2.19                     | 0.41              |
| 54:1:694:U:C2'    | 54:1:695:G:H5''  | 2.50                     | 0.41              |
| 54:1:764:A:O2'    | 54:1:765:C:H5'   | 2.21                     | 0.41              |
| 54:1:891:G:H2'    | 54:1:892:A:C8    | 2.53                     | 0.41              |
| 54:1:1054:A:H61   | 54:1:1105:U:H3   | 1.67                     | 0.41              |
| 54:1:1677:A:H2'   | 54:1:1678:A:O4'  | 2.20                     | 0.41              |
| 54:1:2012:G:H8    | 54:1:2012:G:O5'  | 2.03                     | 0.41              |
| 54:1:2141:G:H2'   | 54:1:2142:A:C8   | 2.53                     | 0.41              |
| 54:1:2671:G:O2'   | 54:1:2672:U:H5'  | 2.21                     | 0.41              |
| 54:1:2898:U:H2'   | 54:1:2899:A:H8   | 1.85                     | 0.41              |
| 55:2:95:U:H2'     | 55:2:96:G:C8     | 2.54                     | 0.41              |
| 57:6:70:G:H5'     | 57:6:70:G:H8     | 1.85                     | 0.41              |
| 58:4:19:C:H3'     | 58:4:20:C:C5'    | 2.42                     | 0.41              |
| 59:8:402:ALA:O    | 59:8:403:PRO:C   | 2.61                     | 0.41              |
| 59:8:555:LYS:HD3  | 59:8:555:LYS:HA  | 1.94                     | 0.41              |
| 59:8:685:LEU:HD23 | 59:8:686:LYS:HB2 | 2.02                     | 0.41              |
| 1:b:160:TYR:CD1   | 1:b:160:TYR:N    | 2.89                     | 0.41              |
| 3:d:32:VAL:HG11   | 11:l:6:LEU:HD13  | 2.01                     | 0.41              |
| 3:d:111:GLU:OE2   | 3:d:115:GLN:HG2  | 2.20                     | 0.41              |
| 3:d:163:ASN:OD1   | 54:1:323:C:H5''  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 8:i:41:PHE:HA     | 8:i:68:PHE:CZ    | 2.55                     | 0.41              |
| 10:k:71:ARG:HB3   | 10:k:72:PRO:CD   | 2.49                     | 0.41              |
| 11:l:30:THR:O     | 11:l:31:GLY:C    | 2.64                     | 0.41              |
| 13:n:84:GLY:N     | 13:n:85:PRO:HD2  | 2.35                     | 0.41              |
| 20:u:33:VAL:O     | 20:u:64:ILE:HG22 | 2.20                     | 0.41              |
| 25:z:11:SER:OG    | 25:z:12:ALA:N    | 2.53                     | 0.41              |
| 26:A:12:ILE:O     | 26:A:23:LYS:HB2  | 2.19                     | 0.41              |
| 27:B:51:ARG:HB3   | 27:B:51:ARG:HH21 | 1.85                     | 0.41              |
| 28:C:9:LYS:HE3    | 28:C:19:PHE:CD2  | 2.55                     | 0.41              |
| 32:G:220:VAL:HG23 | 32:G:221:ARG:N   | 2.36                     | 0.41              |
| 33:H:79:LYS:O     | 33:H:79:LYS:HG2  | 2.20                     | 0.41              |
| 34:I:36:ALA:HA    | 34:I:41:GLY:CA   | 2.46                     | 0.41              |
| 34:I:68:GLU:O     | 34:I:69:ARG:C    | 2.63                     | 0.41              |
| 34:I:187:ARG:NH2  | 34:I:194:ILE:O   | 2.54                     | 0.41              |
| 38:M:85:TYR:CD2   | 53:3:598:U:H4'   | 2.55                     | 0.41              |
| 42:Q:76:HIS:CE1   | 59:8:425:LYS:NZ  | 2.89                     | 0.41              |
| 43:R:55:LEU:O     | 43:R:59:VAL:HG13 | 2.21                     | 0.41              |
| 53:3:697:U:C2'    | 53:3:698:G:H5'   | 2.49                     | 0.41              |
| 53:3:1106:G:O2'   | 53:3:1107:C:H5'  | 2.20                     | 0.41              |
| 53:3:1158:C:H5''  | 53:3:1159:U:OP2  | 2.21                     | 0.41              |
| 53:3:1399:C:C4    | 53:3:1502:A:N1   | 2.88                     | 0.41              |
| 53:3:1406:U:O2'   | 53:3:1407:C:H5'  | 2.21                     | 0.41              |
| 53:3:1424:U:H2'   | 53:3:1425:U:H6   | 1.85                     | 0.41              |
| 54:1:895:U:H6     | 54:1:895:U:O5'   | 2.03                     | 0.41              |
| 54:1:923:G:O2'    | 54:1:924:G:H5'   | 2.21                     | 0.41              |
| 54:1:973:A:O4'    | 54:1:1188:U:C6   | 2.74                     | 0.41              |
| 54:1:1479:G:O2'   | 54:1:1480:C:H5'  | 2.20                     | 0.41              |
| 54:1:1562:U:H2'   | 54:1:1563:U:O4'  | 2.21                     | 0.41              |
| 54:1:2008:C:H2'   | 54:1:2009:A:H8   | 1.85                     | 0.41              |
| 54:1:2333:A:H4'   | 54:1:2334:U:O5'  | 2.20                     | 0.41              |
| 54:1:2423:U:H5'   | 54:1:2424:C:OP1  | 2.20                     | 0.41              |
| 54:1:2648:G:H2'   | 54:1:2649:C:H6   | 1.85                     | 0.41              |
| 55:2:119:A:H2'    | 55:2:120:A:O4'   | 2.21                     | 0.41              |
| 59:8:87:ILE:HG22  | 59:8:88:ASP:N    | 2.35                     | 0.41              |
| 59:8:322:PHE:CD1  | 59:8:322:PHE:N   | 2.88                     | 0.41              |
| 1:b:54:GLY:HA3    | 1:b:216:ARG:HG3  | 2.02                     | 0.41              |
| 2:c:26:VAL:HG13   | 2:c:186:LEU:HD22 | 2.02                     | 0.41              |
| 2:c:49:GLN:HB2    | 2:c:81:GLU:OE2   | 2.21                     | 0.41              |
| 5:f:169:ARG:HG3   | 5:f:169:ARG:HH21 | 1.85                     | 0.41              |
| 8:i:48:ILE:CG1    | 8:i:49:GLU:H     | 2.31                     | 0.41              |
| 13:n:21:PHE:HB3   | 13:n:47:VAL:HG21 | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:z:57:GLU:HG2   | 25:z:57:GLU:O     | 2.20                     | 0.41              |
| 26:A:43:PHE:CD1   | 26:A:44:PHE:N     | 2.88                     | 0.41              |
| 27:B:51:ARG:HB3   | 27:B:53:VAL:HG13  | 2.01                     | 0.41              |
| 32:G:68:PHE:CE2   | 32:G:83:ALA:HA    | 2.56                     | 0.41              |
| 34:I:64:TYR:CE2   | 34:I:93:LEU:HD13  | 2.55                     | 0.41              |
| 38:M:11:THR:HG22  | 38:M:14:ARG:NH2   | 2.35                     | 0.41              |
| 39:N:34:LEU:HD11  | 39:N:47:VAL:HG21  | 2.01                     | 0.41              |
| 44:S:52:ARG:HG3   | 53:3:1317:C:C4    | 2.55                     | 0.41              |
| 45:T:32:THR:HA    | 45:T:62:ARG:NH1   | 2.35                     | 0.41              |
| 49:X:69:LYS:HD2   | 53:3:1320:C:C5'   | 2.44                     | 0.41              |
| 52:a:60:ARG:HH11  | 52:a:60:ARG:HG2   | 1.84                     | 0.41              |
| 52:a:169:GLY:C    | 52:a:170:ILE:HG13 | 2.46                     | 0.41              |
| 53:3:123:U:OP1    | 53:3:312:C:H5'    | 2.20                     | 0.41              |
| 53:3:460:A:H2'    | 53:3:461:A:H8     | 1.86                     | 0.41              |
| 53:3:621:A:H2'    | 53:3:622:A:C8     | 2.56                     | 0.41              |
| 53:3:730:G:H2'    | 53:3:731:G:H5'    | 2.03                     | 0.41              |
| 53:3:823:C:H2'    | 53:3:824:G:H8     | 1.84                     | 0.41              |
| 53:3:900:A:H2'    | 53:3:901:A:C8     | 2.55                     | 0.41              |
| 53:3:1264:U:H3    | 53:3:1271:A:H61   | 1.66                     | 0.41              |
| 53:3:1399:C:N3    | 53:3:1502:A:N1    | 2.68                     | 0.41              |
| 54:1:766:U:H2'    | 54:1:767:U:H6     | 1.86                     | 0.41              |
| 54:1:1417:C:H4'   | 54:1:1587:G:H21   | 1.85                     | 0.41              |
| 54:1:1665:A:O2'   | 54:1:1666:G:H5'   | 2.20                     | 0.41              |
| 54:1:1701:A:H2'   | 54:1:1702:G:H5'   | 2.03                     | 0.41              |
| 54:1:2139:U:H2'   | 54:1:2140:G:C8    | 2.56                     | 0.41              |
| 54:1:2256:G:H2'   | 54:1:2257:U:C6    | 2.56                     | 0.41              |
| 54:1:2470:G:O2'   | 54:1:2471:A:H5'   | 2.21                     | 0.41              |
| 55:2:119:A:C2     | 55:2:120:A:N9     | 2.88                     | 0.41              |
| 59:8:375:LYS:N    | 59:8:375:LYS:HD3  | 2.35                     | 0.41              |
| 4:e:66:ILE:HG13   | 4:e:66:ILE:O      | 2.21                     | 0.41              |
| 4:e:129:MET:SD    | 4:e:129:MET:C     | 3.04                     | 0.41              |
| 5:f:1:SER:HB2     | 54:1:2749:A:H5''  | 2.02                     | 0.41              |
| 5:f:168:VAL:HG12  | 5:f:169:ARG:N     | 2.36                     | 0.41              |
| 19:t:34:VAL:HG11  | 19:t:43:ILE:HD13  | 2.03                     | 0.41              |
| 20:u:42:LYS:HG2   | 20:u:59:GLU:OE1   | 2.20                     | 0.41              |
| 21:v:93:ARG:NH1   | 21:v:93:ARG:HB2   | 2.36                     | 0.41              |
| 31:F:29:ALA:O     | 31:F:31:PRO:HD3   | 2.20                     | 0.41              |
| 32:G:224:ARG:HG3  | 32:G:224:ARG:O    | 2.21                     | 0.41              |
| 34:I:131:ILE:HD12 | 34:I:131:ILE:N    | 2.34                     | 0.41              |
| 36:K:74:LEU:O     | 36:K:78:PHE:HD1   | 2.03                     | 0.41              |
| 41:P:127:ARG:N    | 51:Z:34:ARG:HH21  | 2.19                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:R:70:ARG:HG2   | 43:R:70:ARG:HH11  | 1.86                     | 0.41              |
| 47:V:20:ILE:HG12  | 47:V:21:VAL:N     | 2.36                     | 0.41              |
| 53:3:212:G:O2'    | 53:3:213:G:H5'    | 2.21                     | 0.41              |
| 53:3:252:U:O2     | 53:3:253:A:N7     | 2.54                     | 0.41              |
| 53:3:1125:U:O2    | 53:3:1126:U:H2'   | 2.21                     | 0.41              |
| 53:3:1185:G:O6    | 53:3:1186:G:C2    | 2.73                     | 0.41              |
| 53:3:1223:C:H3'   | 53:3:1224:U:H5''  | 2.03                     | 0.41              |
| 53:3:1404:C:H2'   | 53:3:1405:G:H8    | 1.85                     | 0.41              |
| 54:1:208:C:H2'    | 54:1:209:C:C6     | 2.55                     | 0.41              |
| 54:1:959:A:C6     | 54:1:960:A:C6     | 3.08                     | 0.41              |
| 54:1:1056:G:H8    | 54:1:1056:G:O5'   | 2.03                     | 0.41              |
| 54:1:1783:A:C2    | 54:1:2587:A:C4    | 3.08                     | 0.41              |
| 54:1:1922:G:H2'   | 54:1:1923:U:O4'   | 2.20                     | 0.41              |
| 54:1:2277:G:H2'   | 54:1:2278:A:C5'   | 2.46                     | 0.41              |
| 54:1:2818:U:H4'   | 54:1:2837:A:C4'   | 2.50                     | 0.41              |
| 59:8:29:ARG:HA    | 59:8:29:ARG:NE    | 2.34                     | 0.41              |
| 59:8:475:ARG:NH1  | 59:8:475:ARG:HB3  | 2.35                     | 0.41              |
| 59:8:560:GLN:HE21 | 59:8:602:LYS:HE2  | 1.85                     | 0.41              |
| 9:j:135:GLN:O     | 9:j:136:GLN:HG2   | 2.21                     | 0.41              |
| 12:m:13:HIS:ND1   | 54:1:954:G:H5''   | 2.34                     | 0.41              |
| 12:m:39:GLY:HA3   | 12:m:126:ILE:HG21 | 2.03                     | 0.41              |
| 23:x:2:ARG:O      | 23:x:11:PRO:HD3   | 2.20                     | 0.41              |
| 35:J:23:THR:O     | 35:J:23:THR:HG22  | 2.21                     | 0.41              |
| 35:J:44:ARG:HB3   | 35:J:70:MET:HE3   | 2.03                     | 0.41              |
| 39:N:70:GLY:O     | 39:N:74:GLN:HG3   | 2.20                     | 0.41              |
| 39:N:94:ARG:HH11  | 39:N:94:ARG:HG3   | 1.85                     | 0.41              |
| 45:T:28:VAL:HG13  | 45:T:62:ARG:CG    | 2.50                     | 0.41              |
| 45:T:87:ARG:HG2   | 45:T:87:ARG:HH11  | 1.85                     | 0.41              |
| 46:U:5:ARG:CB     | 53:3:376:G:H5''   | 2.50                     | 0.41              |
| 48:W:12:PHE:C     | 48:W:14:ALA:H     | 2.29                     | 0.41              |
| 52:a:39:VAL:HG13  | 52:a:178:VAL:HG22 | 2.03                     | 0.41              |
| 53:3:210:C:H4'    | 53:3:211:G:N2     | 2.36                     | 0.41              |
| 53:3:458:U:H2'    | 53:3:459:A:H8     | 1.82                     | 0.41              |
| 53:3:609:A:H2'    | 53:3:610:U:C5'    | 2.49                     | 0.41              |
| 53:3:947:G:N3     | 53:3:947:G:H2'    | 2.35                     | 0.41              |
| 53:3:960:U:H4'    | 53:3:961:U:O5'    | 2.21                     | 0.41              |
| 53:3:1114:C:C1'   | 53:3:1115:U:C4    | 3.04                     | 0.41              |
| 53:3:1150:A:H2'   | 53:3:1151:A:N7    | 2.36                     | 0.41              |
| 54:1:510:C:H2'    | 54:1:511:U:H6     | 1.86                     | 0.41              |
| 54:1:1301:A:H2'   | 54:1:1301:A:N3    | 2.35                     | 0.41              |
| 54:1:1686:C:H2'   | 54:1:1687:G:O4'   | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:1:2143:C:H2'   | 54:1:2144:G:O4'   | 2.21                     | 0.41              |
| 54:1:2708:G:O2'   | 54:1:2709:G:H5'   | 2.21                     | 0.41              |
| 59:8:207:ILE:HG21 | 59:8:212:VAL:HA   | 2.03                     | 0.41              |
| 59:8:503:GLY:CA   | 59:8:600:ALA:HB2  | 2.48                     | 0.41              |
| 1:b:106:PRO:HG3   | 1:b:109:LEU:HD22  | 2.03                     | 0.41              |
| 2:c:1:MET:SD      | 2:c:2:ILE:HG12    | 2.61                     | 0.41              |
| 2:c:56:LYS:HE3    | 54:1:2831:G:P     | 2.61                     | 0.41              |
| 2:c:118:PHE:CD2   | 54:1:1654:A:C2    | 3.09                     | 0.41              |
| 7:h:43:LYS:HA     | 7:h:46:ARG:HH11   | 1.84                     | 0.41              |
| 9:j:16:TYR:HE2    | 9:j:52:ASP:CG     | 2.29                     | 0.41              |
| 9:j:39:LYS:HE2    | 9:j:39:LYS:HB3    | 1.94                     | 0.41              |
| 10:k:110:GLU:H    | 10:k:113:MET:HE3  | 1.85                     | 0.41              |
| 13:n:35:LYS:CE    | 13:n:110:MET:HG2  | 2.50                     | 0.41              |
| 13:n:38:LEU:HB3   | 13:n:39:PRO:HD3   | 2.03                     | 0.41              |
| 13:n:64:ARG:HG3   | 13:n:64:ARG:NH2   | 2.35                     | 0.41              |
| 15:p:108:ARG:HD2  | 53:3:1463:U:OP1   | 2.21                     | 0.41              |
| 16:q:23:TYR:HB3   | 16:q:27:ARG:HB3   | 2.03                     | 0.41              |
| 18:s:29:VAL:HG23  | 18:s:69:LEU:C     | 2.45                     | 0.41              |
| 18:s:36:LEU:HD13  | 18:s:47:VAL:HG13  | 2.02                     | 0.41              |
| 19:t:29:THR:HG22  | 19:t:86:THR:HG22  | 2.01                     | 0.41              |
| 19:t:48:GLN:O     | 19:t:52:GLU:HA    | 2.21                     | 0.41              |
| 22:w:17:LEU:HD21  | 22:w:37:ARG:HE    | 1.85                     | 0.41              |
| 22:w:74:LYS:HD3   | 22:w:74:LYS:H     | 1.85                     | 0.41              |
| 28:C:16:THR:HG21  | 28:C:39:ASP:OD2   | 2.20                     | 0.41              |
| 30:E:30:HIS:NE2   | 54:1:2392:A:OP2   | 2.54                     | 0.41              |
| 30:E:44:ARG:N     | 30:E:45:PRO:HD2   | 2.35                     | 0.41              |
| 32:G:13:VAL:HG13  | 32:G:13:VAL:O     | 2.21                     | 0.41              |
| 32:G:34:ARG:HA    | 32:G:34:ARG:NE    | 2.36                     | 0.41              |
| 32:G:209:VAL:O    | 32:G:213:LEU:HG   | 2.21                     | 0.41              |
| 34:I:57:LYS:HA    | 34:I:199:ILE:HD11 | 2.03                     | 0.41              |
| 34:I:202:LEU:HD23 | 34:I:202:LEU:C    | 2.46                     | 0.41              |
| 36:K:91:ARG:HD2   | 36:K:91:ARG:HA    | 1.96                     | 0.41              |
| 36:K:97:THR:HG23  | 36:K:97:THR:O     | 2.20                     | 0.41              |
| 37:L:63:VAL:HG13  | 37:L:66:GLU:OE1   | 2.21                     | 0.41              |
| 37:L:63:VAL:O     | 37:L:63:VAL:HG12  | 2.21                     | 0.41              |
| 38:M:87:ARG:HG3   | 38:M:87:ARG:HH11  | 1.86                     | 0.41              |
| 42:Q:30:ARG:HG2   | 42:Q:30:ARG:HH11  | 1.85                     | 0.41              |
| 42:Q:35:ARG:HB3   | 42:Q:53:ARG:CB    | 2.50                     | 0.41              |
| 42:Q:37:TYR:CD1   | 42:Q:37:TYR:N     | 2.89                     | 0.41              |
| 43:R:104:ASN:O    | 53:3:947:G:OP1    | 2.39                     | 0.41              |
| 46:U:5:ARG:CZ     | 46:U:22:ALA:HB3   | 2.50                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:V:64:ARG:HG3   | 53:3:130:A:C8     | 2.56                     | 0.41              |
| 47:V:78:VAL:HB    | 47:V:79:GLU:OE1   | 2.20                     | 0.41              |
| 48:W:70:THR:OG1   | 48:W:71:ASP:N     | 2.53                     | 0.41              |
| 49:X:8:PRO:HB2    | 49:X:40:PHE:HZ    | 1.85                     | 0.41              |
| 49:X:17:LYS:HB3   | 49:X:30:LEU:CD2   | 2.51                     | 0.41              |
| 49:X:79:TYR:HB3   | 49:X:80:ARG:H     | 1.74                     | 0.41              |
| 52:a:21:TYR:HE1   | 52:a:29:LEU:HD22  | 1.78                     | 0.41              |
| 52:a:46:VAL:HB    | 52:a:171:ILE:HG12 | 2.03                     | 0.41              |
| 53:3:553:A:H2'    | 53:3:554:A:H8     | 1.86                     | 0.41              |
| 53:3:794:A:H2'    | 53:3:795:C:C6     | 2.55                     | 0.41              |
| 53:3:856:C:HO2'   | 53:3:857:C:H5'    | 1.85                     | 0.41              |
| 53:3:946:A:H2'    | 53:3:947:G:C8     | 2.55                     | 0.41              |
| 53:3:1085:U:H3'   | 53:3:1086:U:C5    | 2.56                     | 0.41              |
| 53:3:1091:U:C2    | 53:3:1093:A:C6    | 3.08                     | 0.41              |
| 53:3:1164:G:N2    | 53:3:1165:U:H3    | 2.17                     | 0.41              |
| 53:3:1197:A:C2'   | 53:3:1198:G:H5''  | 2.43                     | 0.41              |
| 53:3:1255:G:O2'   | 53:3:1258:G:H1'   | 2.21                     | 0.41              |
| 53:3:1258:G:H2'   | 53:3:1259:C:H6    | 1.86                     | 0.41              |
| 53:3:1300:G:N1    | 53:3:1335:U:O4'   | 2.53                     | 0.41              |
| 53:3:1357:A:H2'   | 53:3:1358:U:O4'   | 2.20                     | 0.41              |
| 53:3:1466:C:H2'   | 53:3:1467:C:O4'   | 2.20                     | 0.41              |
| 54:1:149:A:H2'    | 54:1:150:U:H6     | 1.84                     | 0.41              |
| 54:1:533:G:H2'    | 54:1:534:U:C6     | 2.56                     | 0.41              |
| 54:1:1218:G:H2'   | 54:1:1219:U:H6    | 1.86                     | 0.41              |
| 54:1:1257:C:H2'   | 54:1:1258:U:C6    | 2.56                     | 0.41              |
| 54:1:1401:G:H2'   | 54:1:1402:U:H6    | 1.83                     | 0.41              |
| 54:1:1501:G:O2'   | 54:1:1502:A:H5'   | 2.20                     | 0.41              |
| 54:1:1530:G:H2'   | 54:1:1531:C:O4'   | 2.20                     | 0.41              |
| 54:1:1601:G:O2'   | 54:1:1602:U:H5'   | 2.20                     | 0.41              |
| 54:1:1669:A:H5''  | 54:1:2550:G:OP1   | 2.21                     | 0.41              |
| 54:1:2024:G:OP2   | 54:1:2034:U:H4'   | 2.20                     | 0.41              |
| 54:1:2245:U:O2    | 54:1:2435:A:C8    | 2.74                     | 0.41              |
| 54:1:2341:G:H2'   | 54:1:2342:C:C6    | 2.56                     | 0.41              |
| 54:1:2363:G:O2'   | 54:1:2364:C:H5'   | 2.20                     | 0.41              |
| 54:1:2860:A:H2'   | 54:1:2861:U:H5'   | 2.03                     | 0.41              |
| 54:1:2888:C:H2'   | 54:1:2889:C:H6    | 1.85                     | 0.41              |
| 56:5:43:U:H2'     | 56:5:44:G:C8      | 2.56                     | 0.41              |
| 57:6:66:C:H2'     | 57:6:67:C:H6      | 1.86                     | 0.41              |
| 59:8:59:ARG:NH1   | 59:8:467:ASP:OD2  | 2.54                     | 0.41              |
| 59:8:235:GLU:O    | 59:8:239:GLY:N    | 2.47                     | 0.41              |
| 59:8:263:LEU:HD11 | 59:8:285:TYR:CB   | 2.51                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 59:8:445:PHE:C   | 59:8:446:ARG:HD2  | 2.46                     | 0.41              |
| 59:8:450:ASP:HB3 | 59:8:455:GLN:H    | 1.85                     | 0.41              |
| 59:8:638:ARG:HE  | 59:8:666:TYR:HD1  | 1.69                     | 0.41              |
| 1:b:29:PHE:CD2   | 1:b:31:PRO:HD2    | 2.56                     | 0.41              |
| 2:c:134:HIS:CE1  | 54:1:1675:C:N3    | 2.89                     | 0.41              |
| 3:d:99:LYS:HD3   | 54:1:601:C:H4'    | 2.03                     | 0.41              |
| 3:d:106:LYS:HA   | 3:d:200:LEU:HD21  | 2.01                     | 0.41              |
| 4:e:151:LEU:C    | 4:e:151:LEU:HD12  | 2.46                     | 0.41              |
| 7:h:27:VAL:HG12  | 7:h:83:ALA:HB3    | 2.02                     | 0.41              |
| 8:i:4:VAL:HG22   | 8:i:7:TYR:OH      | 2.21                     | 0.41              |
| 9:j:42:ALA:O     | 16:q:63:ARG:HD2   | 2.21                     | 0.41              |
| 9:j:57:LEU:C     | 9:j:57:LEU:HD12   | 2.46                     | 0.41              |
| 12:m:62:LYS:HD2  | 12:m:64:TRP:CZ2   | 2.56                     | 0.41              |
| 14:o:30:ARG:HG2  | 14:o:30:ARG:HH11  | 1.86                     | 0.41              |
| 15:p:8:GLU:OE1   | 15:p:54:LEU:HD23  | 2.21                     | 0.41              |
| 17:r:20:VAL:HG12 | 17:r:21:ARG:N     | 2.36                     | 0.41              |
| 33:H:107:LYS:HD3 | 33:H:110:LEU:CD1  | 2.51                     | 0.41              |
| 33:H:107:LYS:CB  | 33:H:110:LEU:HD12 | 2.50                     | 0.41              |
| 34:I:119:HIS:CE1 | 53:3:437:U:O2     | 2.74                     | 0.41              |
| 40:O:38:GLY:N    | 53:3:1124:G:OP1   | 2.54                     | 0.41              |
| 42:Q:49:ARG:NH1  | 53:3:521:G:N7     | 2.59                     | 0.41              |
| 43:R:53:ASP:HA   | 43:R:56:ARG:HH11  | 1.84                     | 0.41              |
| 45:T:30:LEU:HD23 | 45:T:30:LEU:C     | 2.46                     | 0.41              |
| 49:X:41:PRO:HA   | 49:X:44:ILE:CD1   | 2.51                     | 0.41              |
| 53:3:15:G:N2     | 53:3:16:A:H1'     | 2.36                     | 0.41              |
| 53:3:144:G:O2'   | 53:3:145:G:H5'    | 2.21                     | 0.41              |
| 53:3:304:U:H2'   | 53:3:305:G:C8     | 2.55                     | 0.41              |
| 53:3:1056:U:OP1  | 53:3:1196:A:H2    | 2.04                     | 0.41              |
| 53:3:1168:U:O5'  | 53:3:1169:A:C8    | 2.74                     | 0.41              |
| 53:3:1352:C:H2'  | 53:3:1353:G:C8    | 2.55                     | 0.41              |
| 54:1:207:A:H2'   | 54:1:208:C:O4'    | 2.22                     | 0.41              |
| 54:1:279:A:C2'   | 54:1:280:U:H5'    | 2.50                     | 0.41              |
| 54:1:543:G:H8    | 54:1:543:G:H5'    | 1.86                     | 0.41              |
| 54:1:560:C:H2'   | 54:1:561:G:O4'    | 2.21                     | 0.41              |
| 54:1:1213:A:N6   | 54:1:1236:G:O2'   | 2.54                     | 0.41              |
| 54:1:1313:U:O2   | 54:1:1313:U:C2'   | 2.69                     | 0.41              |
| 54:1:1524:G:H2'  | 54:1:1525:A:H8    | 1.86                     | 0.41              |
| 54:1:2114:A:C5   | 54:1:2115:G:H1'   | 2.56                     | 0.41              |
| 59:8:637:ARG:C   | 59:8:639:ARG:H    | 2.29                     | 0.41              |
| 2:c:148:GLN:HB3  | 54:1:2574:G:O2'   | 2.21                     | 0.40              |
| 6:g:9:VAL:C      | 6:g:11:ASN:N      | 2.80                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:i:9:LYS:HE3    | 54:1:1070:A:C2    | 2.56                     | 0.40              |
| 8:i:52:LEU:C     | 8:i:54:ILE:HD12   | 2.45                     | 0.40              |
| 9:j:69:ARG:O     | 9:j:89:PHE:HB3    | 2.21                     | 0.40              |
| 18:s:84:ARG:HG2  | 18:s:84:ARG:NH2   | 2.37                     | 0.40              |
| 19:t:2:ILE:O     | 19:t:5:GLU:HB3    | 2.22                     | 0.40              |
| 20:u:98:ASN:O    | 20:u:100:GLU:N    | 2.54                     | 0.40              |
| 29:D:14:ARG:HG3  | 29:D:14:ARG:HH21  | 1.87                     | 0.40              |
| 32:G:43:GLU:CD   | 32:G:43:GLU:N     | 2.80                     | 0.40              |
| 32:G:111:LYS:C   | 32:G:111:LYS:HD3  | 2.46                     | 0.40              |
| 34:I:104:MET:SD  | 34:I:170:LEU:HB2  | 2.61                     | 0.40              |
| 35:J:121:ASN:HB3 | 35:J:122:VAL:H    | 1.61                     | 0.40              |
| 36:K:3:HIS:N     | 36:K:92:THR:HG22  | 2.18                     | 0.40              |
| 39:N:39:GLY:HA2  | 39:N:44:ARG:HB2   | 2.02                     | 0.40              |
| 41:P:123:PRO:HG2 | 51:Z:33:ARG:HB3   | 2.02                     | 0.40              |
| 43:R:87:GLY:O    | 43:R:91:ARG:N     | 2.41                     | 0.40              |
| 43:R:92:ARG:CB   | 43:R:92:ARG:HH11  | 2.33                     | 0.40              |
| 45:T:80:LEU:HA   | 45:T:83:ARG:CG    | 2.51                     | 0.40              |
| 46:U:12:LYS:HE3  | 53:3:393:A:OP2    | 2.20                     | 0.40              |
| 48:W:12:PHE:CG   | 48:W:13:THR:N     | 2.89                     | 0.40              |
| 52:a:8:MET:O     | 52:a:12:ARG:HG3   | 2.21                     | 0.40              |
| 52:a:42:VAL:HG21 | 52:a:185:LEU:CD1  | 2.50                     | 0.40              |
| 53:3:45:G:H2'    | 53:3:46:G:H8      | 1.86                     | 0.40              |
| 53:3:1264:U:H2'  | 53:3:1265:C:C6    | 2.56                     | 0.40              |
| 53:3:1287:A:C2   | 53:3:1353:G:H1'   | 2.56                     | 0.40              |
| 54:1:967:U:H2'   | 54:1:968:C:C6     | 2.56                     | 0.40              |
| 54:1:1280:G:O2'  | 54:1:1281:G:H5'   | 2.20                     | 0.40              |
| 54:1:1475:G:HO2' | 54:1:1476:U:H6    | 1.58                     | 0.40              |
| 54:1:1906:G:C3'  | 54:1:1907:G:H5''  | 2.50                     | 0.40              |
| 54:1:1999:C:H5'' | 54:1:2723:C:O2'   | 2.21                     | 0.40              |
| 54:1:2247:A:H2'  | 54:1:2248:C:C6    | 2.56                     | 0.40              |
| 54:1:2691:C:H2'  | 54:1:2692:G:H8    | 1.85                     | 0.40              |
| 54:1:2733:A:O2'  | 54:1:2734:A:H5'   | 2.21                     | 0.40              |
| 56:5:63:U:O2'    | 56:5:64:C:H5'     | 2.21                     | 0.40              |
| 59:8:134:LYS:HE2 | 59:8:134:LYS:HB2  | 1.92                     | 0.40              |
| 59:8:171:LEU:HB3 | 59:8:183:VAL:HG12 | 2.03                     | 0.40              |
| 13:n:2:ARG:O     | 13:n:2:ARG:HG2    | 2.21                     | 0.40              |
| 14:o:87:ILE:H    | 14:o:87:ILE:CD1   | 2.27                     | 0.40              |
| 20:u:80:ASP:OD2  | 20:u:95:PHE:HB3   | 2.21                     | 0.40              |
| 32:G:139:GLU:O   | 32:G:143:LEU:HD13 | 2.20                     | 0.40              |
| 33:H:63:ILE:HG23 | 33:H:63:ILE:O     | 2.21                     | 0.40              |
| 33:H:86:LEU:HB3  | 33:H:100:ILE:CD1  | 2.52                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:I:8:LEU:HD23   | 34:I:31:CYS:HB3   | 2.02                     | 0.40              |
| 34:I:159:GLU:O    | 34:I:162:GLU:HG2  | 2.22                     | 0.40              |
| 38:M:19:ALA:HB3   | 38:M:21:LYS:HG3   | 2.02                     | 0.40              |
| 44:S:52:ARG:HH11  | 53:3:1317:C:N4    | 2.00                     | 0.40              |
| 46:U:1:MET:O      | 46:U:24:SER:N     | 2.53                     | 0.40              |
| 50:Y:72:ALA:O     | 50:Y:76:ALA:N     | 2.44                     | 0.40              |
| 52:a:171:ILE:HD11 | 52:a:192:LEU:HD21 | 2.02                     | 0.40              |
| 53:3:38:G:H4'     | 53:3:547:A:C6     | 2.57                     | 0.40              |
| 53:3:47:C:H4'     | 53:3:48:C:C5'     | 2.52                     | 0.40              |
| 53:3:1166:G:C8    | 53:3:1166:G:H5''  | 2.56                     | 0.40              |
| 53:3:1238:A:H2'   | 53:3:1238:A:N3    | 2.36                     | 0.40              |
| 54:1:57:C:H2'     | 54:1:58:G:O4'     | 2.22                     | 0.40              |
| 54:1:181:A:H2'    | 54:1:182:A:H8     | 1.86                     | 0.40              |
| 54:1:511:U:H2'    | 54:1:512:G:H5'    | 2.02                     | 0.40              |
| 54:1:991:C:H5'    | 54:1:1185:G:H2'   | 2.03                     | 0.40              |
| 54:1:1022:G:N2    | 54:1:1142:A:C2    | 2.90                     | 0.40              |
| 54:1:2302:U:H2'   | 54:1:2303:G:C8    | 2.56                     | 0.40              |
| 59:8:10:TYR:HE1   | 59:8:83:ARG:NE    | 2.19                     | 0.40              |
| 59:8:18:HIS:ND1   | 59:8:19:ILE:N     | 2.69                     | 0.40              |
| 59:8:320:LEU:HA   | 59:8:396:THR:HA   | 2.02                     | 0.40              |
| 1:b:204:LEU:HB2   | 54:1:1791:A:O3'   | 2.21                     | 0.40              |
| 2:c:152:PRO:HG2   | 2:c:153:GLY:N     | 2.36                     | 0.40              |
| 3:d:88:ARG:HD3    | 3:d:88:ARG:HA     | 1.96                     | 0.40              |
| 5:f:34:ARG:CZ     | 5:f:70:LEU:HD13   | 2.51                     | 0.40              |
| 5:f:82:PHE:HB3    | 5:f:140:ILE:HD13  | 2.03                     | 0.40              |
| 7:h:33:VAL:HG23   | 7:h:33:VAL:O      | 2.22                     | 0.40              |
| 7:h:61:ARG:O      | 54:1:1046:A:O2'   | 2.35                     | 0.40              |
| 9:j:55:ILE:HD11   | 9:j:130:HIS:CB    | 2.51                     | 0.40              |
| 9:j:129:GLU:OE2   | 9:j:130:HIS:O     | 2.40                     | 0.40              |
| 11:l:82:LEU:HD11  | 11:l:90:VAL:HG21  | 2.04                     | 0.40              |
| 12:m:136:MET:HE2  | 21:v:77:VAL:HG12  | 2.02                     | 0.40              |
| 16:q:112:ALA:O    | 16:q:116:LEU:N    | 2.42                     | 0.40              |
| 20:u:21:ARG:HD3   | 20:u:72:PHE:CE2   | 2.55                     | 0.40              |
| 26:A:58:ASP:HB2   | 49:X:20:LYS:NZ    | 2.37                     | 0.40              |
| 32:G:39:ILE:HG22  | 32:G:40:ILE:N     | 2.36                     | 0.40              |
| 32:G:140:LEU:HD23 | 32:G:140:LEU:C    | 2.46                     | 0.40              |
| 33:H:122:GLN:HB3  | 33:H:127:VAL:HG11 | 2.02                     | 0.40              |
| 34:I:49:ASP:O     | 34:I:53:GLN:HG3   | 2.21                     | 0.40              |
| 35:J:10:LEU:HD22  | 35:J:67:ARG:HH21  | 1.86                     | 0.40              |
| 35:J:68:ARG:NH1   | 35:J:68:ARG:CB    | 2.84                     | 0.40              |
| 35:J:96:GLN:HE22  | 35:J:98:ALA:HB2   | 1.87                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:O:10:LEU:HD23  | 40:O:10:LEU:N     | 2.37                     | 0.40              |
| 44:S:98:ALA:HB1   | 44:S:100:TRP:CZ3  | 2.56                     | 0.40              |
| 50:Y:82:ILE:O     | 50:Y:86:ALA:N     | 2.55                     | 0.40              |
| 53:3:17:U:H2'     | 53:3:18:C:C6      | 2.56                     | 0.40              |
| 53:3:971:G:C4     | 53:3:1365:G:H4'   | 2.57                     | 0.40              |
| 53:3:986:U:H2'    | 53:3:987:G:O4'    | 2.21                     | 0.40              |
| 53:3:1252:A:H2'   | 53:3:1253:G:O4'   | 2.22                     | 0.40              |
| 54:1:250:G:C6     | 54:1:251:A:C6     | 3.09                     | 0.40              |
| 54:1:687:C:H2'    | 54:1:688:U:H5'    | 2.03                     | 0.40              |
| 54:1:1053:C:C2'   | 54:1:1054:A:H5''  | 2.51                     | 0.40              |
| 54:1:1312:U:H4'   | 54:1:1313:U:O5'   | 2.21                     | 0.40              |
| 54:1:1666:G:C2'   | 54:1:1667:G:H5'   | 2.51                     | 0.40              |
| 54:1:1924:C:H2'   | 54:1:1925:C:H6    | 1.86                     | 0.40              |
| 54:1:2341:G:H2'   | 54:1:2342:C:H6    | 1.87                     | 0.40              |
| 54:1:2729:G:H2'   | 54:1:2730:C:C6    | 2.56                     | 0.40              |
| 56:5:27:A:H2'     | 56:5:28:C:H6      | 1.85                     | 0.40              |
| 59:8:170:GLN:CB   | 59:8:265:THR:HA   | 2.49                     | 0.40              |
| 59:8:244:THR:HB   | 59:8:247:GLU:HB2  | 2.04                     | 0.40              |
| 59:8:611:VAL:HG21 | 59:8:689:GLU:OE2  | 2.21                     | 0.40              |
| 59:8:638:ARG:HH11 | 59:8:638:ARG:HG2  | 1.87                     | 0.40              |
| 1:b:143:VAL:HB    | 1:b:153:LEU:HB2   | 2.04                     | 0.40              |
| 1:b:211:ARG:HD2   | 1:b:211:ARG:HA    | 1.84                     | 0.40              |
| 4:e:70:ARG:HG2    | 4:e:70:ARG:HH21   | 1.85                     | 0.40              |
| 4:e:72:SER:OG     | 4:e:78:ILE:O      | 2.32                     | 0.40              |
| 5:f:112:VAL:HG13  | 5:f:112:VAL:O     | 2.22                     | 0.40              |
| 8:i:9:LYS:HD2     | 54:1:1061:U:C5'   | 2.52                     | 0.40              |
| 8:i:52:LEU:HA     | 8:i:53:PRO:HD3    | 1.87                     | 0.40              |
| 9:j:37:ARG:HG3    | 9:j:118:MET:CE    | 2.49                     | 0.40              |
| 10:k:79:PHE:CD1   | 15:p:69:VAL:HG22  | 2.57                     | 0.40              |
| 12:m:102:LEU:HD22 | 12:m:102:LEU:N    | 2.36                     | 0.40              |
| 13:n:96:ARG:HB3   | 13:n:114:GLU:HG3  | 2.03                     | 0.40              |
| 15:p:58:PHE:CE1   | 15:p:73:PHE:HB2   | 2.57                     | 0.40              |
| 17:r:6:GLN:HE21   | 17:r:11:GLN:NE2   | 2.18                     | 0.40              |
| 19:t:11:LEU:N     | 19:t:11:LEU:HD12  | 2.37                     | 0.40              |
| 21:v:9:ARG:HB2    | 21:v:39:ALA:HB1   | 2.02                     | 0.40              |
| 21:v:31:TYR:CD2   | 55:2:73:A:N6      | 2.88                     | 0.40              |
| 23:x:65:THR:O     | 23:x:68:ALA:HB3   | 2.21                     | 0.40              |
| 32:G:33:ALA:HB3   | 32:G:37:VAL:CG1   | 2.36                     | 0.40              |
| 32:G:82:ALA:HB2   | 32:G:213:LEU:HD13 | 2.02                     | 0.40              |
| 33:H:5:HIS:ND1    | 33:H:7:ASN:HB3    | 2.36                     | 0.40              |
| 35:J:156:ARG:O    | 35:J:158:LYS:N    | 2.46                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:L:68:VAL:HG23  | 37:L:99:ALA:HB1   | 2.03                     | 0.40              |
| 53:3:687:A:N3     | 53:3:688:G:H1'    | 2.36                     | 0.40              |
| 53:3:892:A:H2'    | 53:3:893:C:H6     | 1.85                     | 0.40              |
| 53:3:958:A:N7     | 53:3:959:A:C6     | 2.89                     | 0.40              |
| 53:3:1105:A:H2'   | 53:3:1106:G:C8    | 2.56                     | 0.40              |
| 53:3:1311:A:C6    | 53:3:1312:G:C8    | 3.10                     | 0.40              |
| 53:3:1365:G:H2'   | 53:3:1365:G:N3    | 2.37                     | 0.40              |
| 54:1:112:U:H2'    | 54:1:113:U:H5'    | 2.03                     | 0.40              |
| 54:1:481:G:H1'    | 54:1:506:G:H22    | 1.81                     | 0.40              |
| 54:1:917:A:H2     | 55:2:79:G:H21     | 1.67                     | 0.40              |
| 54:1:1716:U:H2'   | 54:1:1717:A:C8    | 2.56                     | 0.40              |
| 54:1:1918:A:C2    | 54:1:1919:A:N6    | 2.90                     | 0.40              |
| 54:1:2312:U:C2'   | 54:1:2313:C:H5'   | 2.51                     | 0.40              |
| 54:1:2689:U:O2    | 54:1:2713:U:H5''  | 2.20                     | 0.40              |
| 54:1:2839:G:H2'   | 54:1:2840:C:C6    | 2.56                     | 0.40              |
| 54:1:2839:G:H2'   | 54:1:2840:C:H6    | 1.87                     | 0.40              |
| 59:8:62:THR:HG21  | 59:8:89:THR:HB    | 2.03                     | 0.40              |
| 59:8:406:LEU:HD12 | 59:8:407:GLU:H    | 1.86                     | 0.40              |
| 59:8:431:MET:HE3  | 59:8:435:LEU:HD11 | 2.03                     | 0.40              |
| 59:8:497:LYS:HD3  | 59:8:523:TYR:CD1  | 2.57                     | 0.40              |
| 59:8:632:ILE:HG12 | 59:8:654:ILE:HD13 | 2.02                     | 0.40              |
| 4:e:4:HIS:O       | 4:e:7:TYR:HB3     | 2.22                     | 0.40              |
| 4:e:109:ARG:O     | 4:e:136:ILE:HG22  | 2.21                     | 0.40              |
| 6:g:78:VAL:HG21   | 6:g:103:VAL:HG13  | 2.04                     | 0.40              |
| 13:n:39:PRO:HG2   | 54:1:1651:G:H4'   | 2.04                     | 0.40              |
| 15:p:23:ASP:OD1   | 15:p:89:GLY:N     | 2.55                     | 0.40              |
| 19:t:61:LEU:HD23  | 19:t:61:LEU:N     | 2.36                     | 0.40              |
| 22:w:37:ARG:HD2   | 54:1:2387:U:C1'   | 2.50                     | 0.40              |
| 35:J:75:LEU:HD22  | 35:J:119:VAL:HG13 | 2.03                     | 0.40              |
| 36:K:52:ASN:C     | 36:K:53:LYS:HG3   | 2.47                     | 0.40              |
| 44:S:58:ARG:CZ    | 53:3:979:C:H2'    | 2.51                     | 0.40              |
| 44:S:62:ARG:HG3   | 44:S:67:GLY:HA2   | 2.03                     | 0.40              |
| 45:T:11:VAL:C     | 45:T:13:GLU:H     | 2.30                     | 0.40              |
| 53:3:102:G:C4     | 53:3:103:U:C5     | 3.10                     | 0.40              |
| 53:3:144:G:H2'    | 53:3:145:G:O4'    | 2.21                     | 0.40              |
| 53:3:152:A:C2'    | 53:3:153:C:H5'    | 2.45                     | 0.40              |
| 53:3:156:C:H2'    | 53:3:157:U:O4'    | 2.22                     | 0.40              |
| 53:3:377:G:H2'    | 53:3:378:G:H8     | 1.86                     | 0.40              |
| 53:3:660:C:H2'    | 53:3:661:G:O4'    | 2.22                     | 0.40              |
| 53:3:1162:C:O2'   | 53:3:1163:A:H5'   | 2.21                     | 0.40              |
| 53:3:1168:U:O5'   | 53:3:1169:A:N7    | 2.54                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:3:1517:G:C6    | 53:3:1518:A:C5    | 3.09                     | 0.40              |
| 54:1:361:G:OP2    | 54:1:361:G:H8     | 2.05                     | 0.40              |
| 54:1:1104:C:H2'   | 54:1:1105:U:O4'   | 2.22                     | 0.40              |
| 54:1:1107:G:O2'   | 54:1:1108:U:H5'   | 2.22                     | 0.40              |
| 54:1:1907:G:H2'   | 54:1:1908:C:O4'   | 2.22                     | 0.40              |
| 54:1:1973:G:H2'   | 54:1:1974:C:C6    | 2.57                     | 0.40              |
| 54:1:2180:U:H2'   | 54:1:2181:U:O4'   | 2.21                     | 0.40              |
| 54:1:2631:G:O2'   | 54:1:2632:A:H5'   | 2.22                     | 0.40              |
| 54:1:2655:G:H2'   | 54:1:2664:G:O6    | 2.21                     | 0.40              |
| 54:1:2735:G:O2'   | 54:1:2736:A:H5'   | 2.20                     | 0.40              |
| 54:1:2891:U:H2'   | 54:1:2892:G:C8    | 2.57                     | 0.40              |
| 56:5:44:G:O2'     | 56:5:45:G:H5'     | 2.21                     | 0.40              |
| 59:8:54:GLU:O     | 59:8:55:GLN:C     | 2.64                     | 0.40              |
| 59:8:119:VAL:C    | 59:8:121:PRO:HD2  | 2.46                     | 0.40              |
| 59:8:133:TYR:OH   | 59:8:409:MET:HB2  | 2.22                     | 0.40              |
| 59:8:485:LYS:HD3  | 59:8:485:LYS:HA   | 1.93                     | 0.40              |
| 59:8:493:THR:HG23 | 59:8:611:VAL:HG13 | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | b     | 269/271 (99%) | 232 (86%) | 35 (13%) | 2 (1%)   | 18          | 52  |
| 2   | c     | 207/209 (99%) | 187 (90%) | 20 (10%) | 0        | 100         | 100 |
| 3   | d     | 199/201 (99%) | 176 (88%) | 22 (11%) | 1 (0%)   | 24          | 59  |
| 4   | e     | 175/177 (99%) | 156 (89%) | 17 (10%) | 2 (1%)   | 11          | 43  |
| 5   | f     | 174/176 (99%) | 153 (88%) | 19 (11%) | 2 (1%)   | 11          | 43  |
| 6   | g     | 121/149 (81%) | 97 (80%)  | 19 (16%) | 5 (4%)   | 2           | 17  |
| 7   | h     | 82/131 (63%)  | 62 (76%)  | 16 (20%) | 4 (5%)   | 1           | 13  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 8   | i     | 72/141 (51%)  | 54 (75%)  | 17 (24%) | 1 (1%)   | 9           | 39  |
| 9   | j     | 140/142 (99%) | 128 (91%) | 12 (9%)  | 0        | 100         | 100 |
| 10  | k     | 120/122 (98%) | 100 (83%) | 15 (12%) | 5 (4%)   | 2           | 16  |
| 11  | l     | 141/143 (99%) | 116 (82%) | 23 (16%) | 2 (1%)   | 9           | 39  |
| 12  | m     | 134/136 (98%) | 120 (90%) | 13 (10%) | 1 (1%)   | 18          | 52  |
| 13  | n     | 118/120 (98%) | 101 (86%) | 16 (14%) | 1 (1%)   | 16          | 50  |
| 14  | o     | 114/116 (98%) | 99 (87%)  | 15 (13%) | 0        | 100         | 100 |
| 15  | p     | 112/114 (98%) | 98 (88%)  | 13 (12%) | 1 (1%)   | 14          | 47  |
| 16  | q     | 115/117 (98%) | 109 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 17  | r     | 101/103 (98%) | 82 (81%)  | 18 (18%) | 1 (1%)   | 12          | 45  |
| 18  | s     | 108/110 (98%) | 91 (84%)  | 17 (16%) | 0        | 100         | 100 |
| 19  | t     | 91/93 (98%)   | 85 (93%)  | 6 (7%)   | 0        | 100         | 100 |
| 20  | u     | 100/102 (98%) | 82 (82%)  | 17 (17%) | 1 (1%)   | 12          | 45  |
| 21  | v     | 92/94 (98%)   | 82 (89%)  | 9 (10%)  | 1 (1%)   | 11          | 43  |
| 22  | w     | 73/75 (97%)   | 64 (88%)  | 9 (12%)  | 0        | 100         | 100 |
| 23  | x     | 75/77 (97%)   | 65 (87%)  | 10 (13%) | 0        | 100         | 100 |
| 24  | y     | 61/63 (97%)   | 54 (88%)  | 7 (12%)  | 0        | 100         | 100 |
| 25  | z     | 56/58 (97%)   | 54 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 26  | A     | 64/66 (97%)   | 45 (70%)  | 17 (27%) | 2 (3%)   | 3           | 22  |
| 27  | B     | 54/56 (96%)   | 48 (89%)  | 6 (11%)  | 0        | 100         | 100 |
| 28  | C     | 48/50 (96%)   | 40 (83%)  | 8 (17%)  | 0        | 100         | 100 |
| 29  | D     | 44/46 (96%)   | 38 (86%)  | 6 (14%)  | 0        | 100         | 100 |
| 30  | E     | 62/64 (97%)   | 50 (81%)  | 9 (14%)  | 3 (5%)   | 2           | 14  |
| 31  | F     | 36/38 (95%)   | 30 (83%)  | 6 (17%)  | 0        | 100         | 100 |
| 32  | G     | 216/225 (96%) | 175 (81%) | 39 (18%) | 2 (1%)   | 14          | 47  |
| 33  | H     | 204/206 (99%) | 181 (89%) | 22 (11%) | 1 (0%)   | 24          | 59  |
| 34  | I     | 203/205 (99%) | 173 (85%) | 28 (14%) | 2 (1%)   | 12          | 45  |
| 35  | J     | 155/157 (99%) | 128 (83%) | 20 (13%) | 7 (4%)   | 2           | 15  |
| 36  | K     | 98/100 (98%)  | 78 (80%)  | 14 (14%) | 6 (6%)   | 1           | 9   |
| 37  | L     | 149/151 (99%) | 128 (86%) | 20 (13%) | 1 (1%)   | 18          | 52  |
| 38  | M     | 127/129 (98%) | 114 (90%) | 13 (10%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 39  | N     | 125/127 (98%)   | 93 (74%)   | 26 (21%)  | 6 (5%)   | 2           | 14  |
| 40  | O     | 96/98 (98%)     | 72 (75%)   | 19 (20%)  | 5 (5%)   | 1           | 12  |
| 41  | P     | 114/116 (98%)   | 96 (84%)   | 15 (13%)  | 3 (3%)   | 4           | 26  |
| 42  | Q     | 121/123 (98%)   | 95 (78%)   | 23 (19%)  | 3 (2%)   | 4           | 27  |
| 43  | R     | 112/114 (98%)   | 89 (80%)   | 19 (17%)  | 4 (4%)   | 2           | 19  |
| 44  | S     | 98/100 (98%)    | 81 (83%)   | 13 (13%)  | 4 (4%)   | 2           | 17  |
| 45  | T     | 86/88 (98%)     | 69 (80%)   | 16 (19%)  | 1 (1%)   | 10          | 42  |
| 46  | U     | 80/82 (98%)     | 66 (82%)   | 14 (18%)  | 0        | 100         | 100 |
| 47  | V     | 78/80 (98%)     | 59 (76%)   | 17 (22%)  | 2 (3%)   | 4           | 26  |
| 48  | W     | 63/65 (97%)     | 51 (81%)   | 11 (18%)  | 1 (2%)   | 7           | 36  |
| 49  | X     | 77/79 (98%)     | 58 (75%)   | 19 (25%)  | 0        | 100         | 100 |
| 50  | Y     | 83/85 (98%)     | 75 (90%)   | 8 (10%)   | 0        | 100         | 100 |
| 51  | Z     | 63/65 (97%)     | 35 (56%)   | 25 (40%)  | 3 (5%)   | 2           | 14  |
| 52  | a     | 130/223 (58%)   | 118 (91%)  | 10 (8%)   | 2 (2%)   | 8           | 37  |
| 59  | 8     | 681/711 (96%)   | 561 (82%)  | 103 (15%) | 17 (2%)  | 4           | 27  |
| All | All   | 6517/6889 (95%) | 5493 (84%) | 919 (14%) | 105 (2%) | 10          | 36  |

All (105) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | g     | 14  | SER  |
| 10  | k     | 92  | GLU  |
| 17  | r     | 54  | VAL  |
| 20  | u     | 99  | SER  |
| 30  | E     | 31  | ILE  |
| 35  | J     | 87  | VAL  |
| 35  | J     | 122 | VAL  |
| 39  | N     | 90  | ASP  |
| 44  | S     | 20  | PHE  |
| 44  | S     | 54  | SER  |
| 45  | T     | 46  | LYS  |
| 47  | V     | 49  | ASN  |
| 51  | Z     | 9   | GLU  |
| 51  | Z     | 37  | TYR  |
| 59  | 8     | 122 | GLN  |
| 59  | 8     | 586 | VAL  |
| 59  | 8     | 624 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59  | 8     | 628 | THR  |
| 1   | b     | 232 | GLY  |
| 6   | g     | 12  | LEU  |
| 7   | h     | 32  | GLY  |
| 10  | k     | 35  | VAL  |
| 13  | n     | 71  | ARG  |
| 32  | G     | 19  | THR  |
| 32  | G     | 87  | ASP  |
| 35  | J     | 93  | VAL  |
| 39  | N     | 57  | VAL  |
| 40  | O     | 58  | ASN  |
| 40  | O     | 89  | ARG  |
| 41  | P     | 89  | GLY  |
| 43  | R     | 105 | ALA  |
| 47  | V     | 34  | GLY  |
| 48  | W     | 17  | VAL  |
| 59  | 8     | 121 | PRO  |
| 59  | 8     | 302 | GLY  |
| 59  | 8     | 425 | LYS  |
| 59  | 8     | 649 | VAL  |
| 59  | 8     | 664 | PHE  |
| 3   | d     | 82  | GLY  |
| 5   | f     | 45  | ALA  |
| 5   | f     | 174 | LYS  |
| 6   | g     | 9   | VAL  |
| 6   | g     | 89  | LYS  |
| 7   | h     | 81  | LEU  |
| 10  | k     | 106 | GLU  |
| 11  | l     | 31  | GLY  |
| 35  | J     | 25  | LYS  |
| 36  | K     | 52  | ASN  |
| 36  | K     | 54  | LEU  |
| 41  | P     | 125 | LYS  |
| 42  | Q     | 3   | VAL  |
| 42  | Q     | 24  | GLU  |
| 43  | R     | 100 | ARG  |
| 52  | a     | 165 | ASN  |
| 59  | 8     | 196 | ALA  |
| 59  | 8     | 242 | GLU  |
| 59  | 8     | 582 | SER  |
| 59  | 8     | 585 | ASP  |
| 4   | e     | 20  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | h     | 58  | THR  |
| 10  | k     | 104 | THR  |
| 26  | A     | 54  | GLY  |
| 30  | E     | 33  | THR  |
| 35  | J     | 97  | PRO  |
| 37  | L     | 111 | GLY  |
| 39  | N     | 120 | ALA  |
| 39  | N     | 125 | GLN  |
| 43  | R     | 65  | GLU  |
| 44  | S     | 61  | ASN  |
| 59  | 8     | 300 | ASP  |
| 59  | 8     | 573 | ASP  |
| 4   | e     | 149 | ARG  |
| 11  | l     | 36  | LYS  |
| 12  | m     | 69  | PRO  |
| 33  | H     | 162 | ALA  |
| 34  | I     | 7   | LYS  |
| 36  | K     | 53  | LYS  |
| 36  | K     | 92  | THR  |
| 39  | N     | 55  | ASP  |
| 39  | N     | 111 | GLU  |
| 40  | O     | 57  | VAL  |
| 41  | P     | 77  | GLY  |
| 44  | S     | 60  | ARG  |
| 52  | a     | 68  | GLY  |
| 6   | g     | 94  | ILE  |
| 8   | i     | 4   | VAL  |
| 15  | p     | 113 | LEU  |
| 21  | v     | 93  | ARG  |
| 34  | I     | 182 | LYS  |
| 35  | J     | 50  | GLY  |
| 40  | O     | 43  | PRO  |
| 7   | h     | 79  | PRO  |
| 36  | K     | 12  | PRO  |
| 42  | Q     | 117 | GLY  |
| 26  | A     | 51  | VAL  |
| 35  | J     | 157 | GLY  |
| 40  | O     | 39  | PRO  |
| 30  | E     | 62  | PRO  |
| 51  | Z     | 10  | PRO  |
| 1   | b     | 205 | GLY  |
| 43  | R     | 6   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59  | 8     | 404 | ILE  |
| 59  | 8     | 547 | GLY  |
| 10  | k     | 93  | GLN  |
| 36  | K     | 18  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | b     | 216/216 (100%) | 212 (98%)  | 4 (2%)   | 50          | 73  |
| 2   | c     | 164/164 (100%) | 162 (99%)  | 2 (1%)   | 63          | 79  |
| 3   | d     | 165/165 (100%) | 164 (99%)  | 1 (1%)   | 78          | 84  |
| 4   | e     | 148/148 (100%) | 145 (98%)  | 3 (2%)   | 48          | 72  |
| 5   | f     | 137/137 (100%) | 137 (100%) | 0        | 100         | 100 |
| 6   | g     | 98/114 (86%)   | 98 (100%)  | 0        | 100         | 100 |
| 7   | h     | 66/100 (66%)   | 66 (100%)  | 0        | 100         | 100 |
| 8   | i     | 60/109 (55%)   | 60 (100%)  | 0        | 100         | 100 |
| 9   | j     | 116/116 (100%) | 116 (100%) | 0        | 100         | 100 |
| 10  | k     | 103/103 (100%) | 97 (94%)   | 6 (6%)   | 18          | 51  |
| 11  | l     | 102/102 (100%) | 102 (100%) | 0        | 100         | 100 |
| 12  | m     | 109/109 (100%) | 108 (99%)  | 1 (1%)   | 70          | 81  |
| 13  | n     | 100/100 (100%) | 98 (98%)   | 2 (2%)   | 48          | 72  |
| 14  | o     | 86/86 (100%)   | 84 (98%)   | 2 (2%)   | 44          | 70  |
| 15  | p     | 99/99 (100%)   | 96 (97%)   | 3 (3%)   | 36          | 66  |
| 16  | q     | 89/89 (100%)   | 89 (100%)  | 0        | 100         | 100 |
| 17  | r     | 84/84 (100%)   | 84 (100%)  | 0        | 100         | 100 |
| 18  | s     | 93/93 (100%)   | 93 (100%)  | 0        | 100         | 100 |
| 19  | t     | 80/80 (100%)   | 80 (100%)  | 0        | 100         | 100 |
| 20  | u     | 83/83 (100%)   | 83 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 21  | v     | 78/78 (100%)   | 77 (99%)   | 1 (1%)   | 61          | 78  |
| 22  | w     | 57/57 (100%)   | 57 (100%)  | 0        | 100         | 100 |
| 23  | x     | 67/67 (100%)   | 67 (100%)  | 0        | 100         | 100 |
| 24  | y     | 55/55 (100%)   | 55 (100%)  | 0        | 100         | 100 |
| 25  | z     | 48/48 (100%)   | 47 (98%)   | 1 (2%)   | 47          | 71  |
| 26  | A     | 59/59 (100%)   | 57 (97%)   | 2 (3%)   | 32          | 64  |
| 27  | B     | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 28  | C     | 45/45 (100%)   | 44 (98%)   | 1 (2%)   | 45          | 71  |
| 29  | D     | 38/38 (100%)   | 38 (100%)  | 0        | 100         | 100 |
| 30  | E     | 51/51 (100%)   | 48 (94%)   | 3 (6%)   | 18          | 50  |
| 31  | F     | 34/34 (100%)   | 33 (97%)   | 1 (3%)   | 37          | 67  |
| 32  | G     | 180/186 (97%)  | 179 (99%)  | 1 (1%)   | 78          | 84  |
| 33  | H     | 170/170 (100%) | 166 (98%)  | 4 (2%)   | 43          | 70  |
| 34  | I     | 172/172 (100%) | 171 (99%)  | 1 (1%)   | 78          | 84  |
| 35  | J     | 119/119 (100%) | 113 (95%)  | 6 (5%)   | 22          | 55  |
| 36  | K     | 87/87 (100%)   | 84 (97%)   | 3 (3%)   | 32          | 64  |
| 37  | L     | 124/124 (100%) | 124 (100%) | 0        | 100         | 100 |
| 38  | M     | 104/104 (100%) | 103 (99%)  | 1 (1%)   | 68          | 80  |
| 39  | N     | 105/105 (100%) | 105 (100%) | 0        | 100         | 100 |
| 40  | O     | 86/86 (100%)   | 78 (91%)   | 8 (9%)   | 8           | 33  |
| 41  | P     | 89/89 (100%)   | 85 (96%)   | 4 (4%)   | 24          | 58  |
| 42  | Q     | 103/103 (100%) | 101 (98%)  | 2 (2%)   | 50          | 73  |
| 43  | R     | 92/92 (100%)   | 85 (92%)   | 7 (8%)   | 12          | 42  |
| 44  | S     | 83/83 (100%)   | 80 (96%)   | 3 (4%)   | 31          | 63  |
| 45  | T     | 76/76 (100%)   | 74 (97%)   | 2 (3%)   | 40          | 69  |
| 46  | U     | 65/65 (100%)   | 64 (98%)   | 1 (2%)   | 57          | 76  |
| 47  | V     | 74/74 (100%)   | 74 (100%)  | 0        | 100         | 100 |
| 48  | W     | 56/56 (100%)   | 55 (98%)   | 1 (2%)   | 51          | 74  |
| 49  | X     | 70/70 (100%)   | 69 (99%)   | 1 (1%)   | 59          | 77  |
| 50  | Y     | 65/65 (100%)   | 64 (98%)   | 1 (2%)   | 57          | 76  |
| 51  | Z     | 55/55 (100%)   | 54 (98%)   | 1 (2%)   | 51          | 74  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 52  | a     | 110/174 (63%)   | 109 (99%)  | 1 (1%)   | 70          | 81 |
| 59  | 8     | 566/585 (97%)   | 550 (97%)  | 16 (3%)  | 38          | 68 |
| All | All   | 5428/5616 (97%) | 5331 (98%) | 97 (2%)  | 51          | 74 |

All (97) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 52  | HIS  |
| 1   | b     | 129 | LEU  |
| 1   | b     | 145 | MET  |
| 1   | b     | 270 | ARG  |
| 2   | c     | 1   | MET  |
| 2   | c     | 146 | ILE  |
| 3   | d     | 1   | MET  |
| 4   | e     | 71  | LYS  |
| 4   | e     | 84  | ILE  |
| 4   | e     | 134 | GLN  |
| 10  | k     | 1   | MET  |
| 10  | k     | 58  | LEU  |
| 10  | k     | 65  | THR  |
| 10  | k     | 93  | GLN  |
| 10  | k     | 104 | THR  |
| 10  | k     | 122 | VAL  |
| 12  | m     | 97  | GLN  |
| 13  | n     | 12  | ARG  |
| 13  | n     | 37  | THR  |
| 14  | o     | 31  | THR  |
| 14  | o     | 112 | GLU  |
| 15  | p     | 3   | ILE  |
| 15  | p     | 30  | TRP  |
| 15  | p     | 65  | ASN  |
| 21  | v     | 12  | GLN  |
| 25  | z     | 16  | LEU  |
| 26  | A     | 27  | THR  |
| 26  | A     | 58  | ASP  |
| 28  | C     | 4   | ILE  |
| 30  | E     | 30  | HIS  |
| 30  | E     | 32  | LEU  |
| 30  | E     | 61  | LEU  |
| 31  | F     | 23  | ILE  |
| 32  | G     | 131 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | H     | 153 | SER  |
| 33  | H     | 156 | LEU  |
| 33  | H     | 165 | GLU  |
| 33  | H     | 169 | GLU  |
| 34  | I     | 130 | ASN  |
| 35  | J     | 28  | ARG  |
| 35  | J     | 55  | VAL  |
| 35  | J     | 97  | PRO  |
| 35  | J     | 123 | LEU  |
| 35  | J     | 133 | ILE  |
| 35  | J     | 147 | ASN  |
| 36  | K     | 12  | PRO  |
| 36  | K     | 58  | HIS  |
| 36  | K     | 86  | ARG  |
| 38  | M     | 60  | LEU  |
| 40  | O     | 20  | GLN  |
| 40  | O     | 36  | VAL  |
| 40  | O     | 40  | ILE  |
| 40  | O     | 42  | LEU  |
| 40  | O     | 43  | PRO  |
| 40  | O     | 69  | THR  |
| 40  | O     | 73  | LEU  |
| 40  | O     | 75  | ASP  |
| 41  | P     | 30  | ILE  |
| 41  | P     | 34  | THR  |
| 41  | P     | 82  | GLU  |
| 41  | P     | 118 | ASN  |
| 42  | Q     | 19  | ASN  |
| 42  | Q     | 102 | ASP  |
| 43  | R     | 64  | VAL  |
| 43  | R     | 90  | HIS  |
| 43  | R     | 95  | PRO  |
| 43  | R     | 97  | ARG  |
| 43  | R     | 99  | GLN  |
| 43  | R     | 104 | ASN  |
| 43  | R     | 107 | THR  |
| 44  | S     | 2   | LYS  |
| 44  | S     | 5   | MET  |
| 44  | S     | 55  | SER  |
| 45  | T     | 27  | GLN  |
| 45  | T     | 86  | LEU  |
| 46  | U     | 46  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | W     | 51  | GLN  |
| 49  | X     | 54  | ARG  |
| 50  | Y     | 29  | THR  |
| 51  | Z     | 11  | PHE  |
| 52  | a     | 217 | THR  |
| 59  | 8     | 19  | ILE  |
| 59  | 8     | 20  | ASP  |
| 59  | 8     | 24  | THR  |
| 59  | 8     | 145 | ASP  |
| 59  | 8     | 220 | GLN  |
| 59  | 8     | 231 | GLU  |
| 59  | 8     | 322 | PHE  |
| 59  | 8     | 334 | THR  |
| 59  | 8     | 442 | ASP  |
| 59  | 8     | 446 | ARG  |
| 59  | 8     | 522 | MET  |
| 59  | 8     | 530 | ASN  |
| 59  | 8     | 587 | ASP  |
| 59  | 8     | 623 | THR  |
| 59  | 8     | 624 | PRO  |
| 59  | 8     | 626 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 24  | HIS  |
| 1   | b     | 45  | ASN  |
| 1   | b     | 59  | GLN  |
| 1   | b     | 196 | ASN  |
| 2   | c     | 134 | HIS  |
| 2   | c     | 149 | ASN  |
| 3   | d     | 30  | GLN  |
| 4   | e     | 20  | ASN  |
| 5   | f     | 87  | GLN  |
| 8   | i     | 42  | ASN  |
| 9   | j     | 58  | ASN  |
| 10  | k     | 5   | GLN  |
| 10  | k     | 13  | ASN  |
| 10  | k     | 88  | ASN  |
| 10  | k     | 90  | ASN  |
| 11  | l     | 4   | ASN  |
| 11  | l     | 38  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | m     | 22  | GLN  |
| 13  | n     | 3   | HIS  |
| 13  | n     | 31  | HIS  |
| 14  | o     | 38  | GLN  |
| 14  | o     | 100 | HIS  |
| 15  | p     | 40  | GLN  |
| 15  | p     | 51  | ASN  |
| 15  | p     | 74  | GLN  |
| 16  | q     | 36  | GLN  |
| 17  | r     | 6   | GLN  |
| 17  | r     | 11  | GLN  |
| 17  | r     | 87  | GLN  |
| 19  | t     | 28  | ASN  |
| 19  | t     | 91  | GLN  |
| 20  | u     | 39  | ASN  |
| 20  | u     | 73  | ASN  |
| 23  | x     | 16  | ASN  |
| 24  | y     | 36  | GLN  |
| 26  | A     | 20  | ASN  |
| 28  | C     | 44  | GLN  |
| 31  | F     | 35  | GLN  |
| 32  | G     | 119 | GLN  |
| 33  | H     | 122 | GLN  |
| 33  | H     | 175 | HIS  |
| 34  | I     | 39  | GLN  |
| 34  | I     | 73  | ASN  |
| 34  | I     | 125 | ASN  |
| 34  | I     | 151 | GLN  |
| 34  | I     | 195 | ASN  |
| 35  | J     | 69  | ASN  |
| 35  | J     | 81  | GLN  |
| 35  | J     | 96  | GLN  |
| 35  | J     | 134 | ASN  |
| 35  | J     | 145 | ASN  |
| 36  | K     | 58  | HIS  |
| 37  | L     | 67  | ASN  |
| 39  | N     | 31  | GLN  |
| 39  | N     | 49  | GLN  |
| 40  | O     | 64  | GLN  |
| 41  | P     | 100 | ASN  |
| 43  | R     | 7   | ASN  |
| 43  | R     | 90  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | S     | 3   | GLN  |
| 44  | S     | 59  | GLN  |
| 45  | T     | 27  | GLN  |
| 45  | T     | 34  | GLN  |
| 46  | U     | 18  | GLN  |
| 47  | V     | 49  | ASN  |
| 49  | X     | 52  | ASN  |
| 50  | Y     | 2   | ASN  |
| 50  | Y     | 20  | ASN  |
| 50  | Y     | 47  | GLN  |
| 50  | Y     | 51  | ASN  |
| 50  | Y     | 69  | ASN  |
| 50  | Y     | 81  | GLN  |
| 51  | Z     | 63  | ASN  |
| 59  | 8     | 55  | GLN  |
| 59  | 8     | 150 | ASN  |
| 59  | 8     | 276 | GLN  |
| 59  | 8     | 369 | ASN  |
| 59  | 8     | 455 | GLN  |
| 59  | 8     | 478 | ASN  |
| 59  | 8     | 645 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 53  | 3     | 1538/1539 (99%) | 214 (13%)         | 17 (1%)         |
| 54  | 1     | 2902/2903 (99%) | 358 (12%)         | 15 (0%)         |
| 55  | 2     | 119/120 (99%)   | 12 (10%)          | 2 (1%)          |
| 56  | 5     | 76/77 (98%)     | 16 (21%)          | 2 (2%)          |
| 57  | 6     | 76/77 (98%)     | 23 (30%)          | 0               |
| 58  | 4     | 15/16 (93%)     | 3 (20%)           | 0               |
| All | All   | 4726/4732 (99%) | 626 (13%)         | 36 (0%)         |

All (626) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 3     | 6   | G    |
| 53  | 3     | 9   | G    |
| 53  | 3     | 22  | G    |
| 53  | 3     | 32  | A    |
| 53  | 3     | 39  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 3     | 48  | C    |
| 53  | 3     | 51  | A    |
| 53  | 3     | 71  | A    |
| 53  | 3     | 82  | G    |
| 53  | 3     | 87  | C    |
| 53  | 3     | 95  | C    |
| 53  | 3     | 100 | G    |
| 53  | 3     | 130 | A    |
| 53  | 3     | 131 | A    |
| 53  | 3     | 144 | G    |
| 53  | 3     | 149 | A    |
| 53  | 3     | 181 | A    |
| 53  | 3     | 183 | C    |
| 53  | 3     | 184 | G    |
| 53  | 3     | 197 | A    |
| 53  | 3     | 209 | U    |
| 53  | 3     | 210 | C    |
| 53  | 3     | 211 | G    |
| 53  | 3     | 226 | G    |
| 53  | 3     | 247 | G    |
| 53  | 3     | 251 | G    |
| 53  | 3     | 253 | A    |
| 53  | 3     | 266 | G    |
| 53  | 3     | 267 | C    |
| 53  | 3     | 281 | G    |
| 53  | 3     | 289 | G    |
| 53  | 3     | 308 | C    |
| 53  | 3     | 316 | C    |
| 53  | 3     | 321 | A    |
| 53  | 3     | 328 | C    |
| 53  | 3     | 345 | C    |
| 53  | 3     | 346 | G    |
| 53  | 3     | 352 | C    |
| 53  | 3     | 354 | G    |
| 53  | 3     | 355 | C    |
| 53  | 3     | 367 | U    |
| 53  | 3     | 372 | C    |
| 53  | 3     | 373 | A    |
| 53  | 3     | 412 | A    |
| 53  | 3     | 413 | G    |
| 53  | 3     | 414 | A    |
| 53  | 3     | 422 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 3     | 429 | U    |
| 53  | 3     | 430 | A    |
| 53  | 3     | 439 | U    |
| 53  | 3     | 462 | G    |
| 53  | 3     | 467 | U    |
| 53  | 3     | 484 | G    |
| 53  | 3     | 486 | U    |
| 53  | 3     | 495 | A    |
| 53  | 3     | 497 | G    |
| 53  | 3     | 518 | C    |
| 53  | 3     | 531 | U    |
| 53  | 3     | 532 | A    |
| 53  | 3     | 533 | A    |
| 53  | 3     | 534 | U    |
| 53  | 3     | 536 | C    |
| 53  | 3     | 537 | G    |
| 53  | 3     | 547 | A    |
| 53  | 3     | 561 | U    |
| 53  | 3     | 572 | A    |
| 53  | 3     | 573 | A    |
| 53  | 3     | 575 | G    |
| 53  | 3     | 576 | C    |
| 53  | 3     | 577 | G    |
| 53  | 3     | 596 | A    |
| 53  | 3     | 607 | A    |
| 53  | 3     | 623 | C    |
| 53  | 3     | 633 | G    |
| 53  | 3     | 665 | A    |
| 53  | 3     | 687 | A    |
| 53  | 3     | 703 | G    |
| 53  | 3     | 724 | G    |
| 53  | 3     | 755 | G    |
| 53  | 3     | 777 | A    |
| 53  | 3     | 815 | A    |
| 53  | 3     | 817 | C    |
| 53  | 3     | 818 | G    |
| 53  | 3     | 819 | A    |
| 53  | 3     | 821 | G    |
| 53  | 3     | 842 | U    |
| 53  | 3     | 843 | U    |
| 53  | 3     | 844 | G    |
| 53  | 3     | 846 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 3     | 851  | G    |
| 53  | 3     | 873  | A    |
| 53  | 3     | 885  | G    |
| 53  | 3     | 890  | G    |
| 53  | 3     | 902  | G    |
| 53  | 3     | 914  | A    |
| 53  | 3     | 926  | G    |
| 53  | 3     | 927  | G    |
| 53  | 3     | 928  | G    |
| 53  | 3     | 929  | G    |
| 53  | 3     | 934  | C    |
| 53  | 3     | 935  | A    |
| 53  | 3     | 946  | A    |
| 53  | 3     | 960  | U    |
| 53  | 3     | 961  | U    |
| 53  | 3     | 966  | G    |
| 53  | 3     | 969  | A    |
| 53  | 3     | 971  | G    |
| 53  | 3     | 975  | A    |
| 53  | 3     | 976  | G    |
| 53  | 3     | 977  | A    |
| 53  | 3     | 979  | C    |
| 53  | 3     | 983  | A    |
| 53  | 3     | 992  | U    |
| 53  | 3     | 993  | G    |
| 53  | 3     | 1004 | A    |
| 53  | 3     | 1020 | G    |
| 53  | 3     | 1028 | C    |
| 53  | 3     | 1031 | C    |
| 53  | 3     | 1033 | G    |
| 53  | 3     | 1034 | G    |
| 53  | 3     | 1053 | G    |
| 53  | 3     | 1054 | C    |
| 53  | 3     | 1055 | A    |
| 53  | 3     | 1061 | G    |
| 53  | 3     | 1062 | U    |
| 53  | 3     | 1064 | G    |
| 53  | 3     | 1065 | U    |
| 53  | 3     | 1066 | C    |
| 53  | 3     | 1079 | G    |
| 53  | 3     | 1080 | A    |
| 53  | 3     | 1081 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 3     | 1086 | U    |
| 53  | 3     | 1092 | A    |
| 53  | 3     | 1093 | A    |
| 53  | 3     | 1094 | G    |
| 53  | 3     | 1095 | U    |
| 53  | 3     | 1101 | A    |
| 53  | 3     | 1115 | U    |
| 53  | 3     | 1116 | U    |
| 53  | 3     | 1118 | U    |
| 53  | 3     | 1119 | C    |
| 53  | 3     | 1121 | U    |
| 53  | 3     | 1122 | U    |
| 53  | 3     | 1123 | U    |
| 53  | 3     | 1124 | G    |
| 53  | 3     | 1125 | U    |
| 53  | 3     | 1126 | U    |
| 53  | 3     | 1127 | G    |
| 53  | 3     | 1136 | C    |
| 53  | 3     | 1137 | C    |
| 53  | 3     | 1138 | G    |
| 53  | 3     | 1139 | G    |
| 53  | 3     | 1148 | U    |
| 53  | 3     | 1149 | C    |
| 53  | 3     | 1159 | U    |
| 53  | 3     | 1160 | G    |
| 53  | 3     | 1165 | U    |
| 53  | 3     | 1166 | G    |
| 53  | 3     | 1167 | A    |
| 53  | 3     | 1168 | U    |
| 53  | 3     | 1169 | A    |
| 53  | 3     | 1182 | G    |
| 53  | 3     | 1183 | U    |
| 53  | 3     | 1184 | G    |
| 53  | 3     | 1190 | G    |
| 53  | 3     | 1191 | A    |
| 53  | 3     | 1196 | A    |
| 53  | 3     | 1198 | G    |
| 53  | 3     | 1201 | A    |
| 53  | 3     | 1202 | U    |
| 53  | 3     | 1212 | U    |
| 53  | 3     | 1225 | A    |
| 53  | 3     | 1238 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 3     | 1240 | U    |
| 53  | 3     | 1241 | G    |
| 53  | 3     | 1258 | G    |
| 53  | 3     | 1260 | G    |
| 53  | 3     | 1275 | A    |
| 53  | 3     | 1278 | G    |
| 53  | 3     | 1280 | A    |
| 53  | 3     | 1282 | C    |
| 53  | 3     | 1286 | U    |
| 53  | 3     | 1287 | A    |
| 53  | 3     | 1300 | G    |
| 53  | 3     | 1303 | C    |
| 53  | 3     | 1305 | G    |
| 53  | 3     | 1306 | A    |
| 53  | 3     | 1308 | U    |
| 53  | 3     | 1313 | U    |
| 53  | 3     | 1317 | C    |
| 53  | 3     | 1346 | A    |
| 53  | 3     | 1347 | G    |
| 53  | 3     | 1363 | A    |
| 53  | 3     | 1378 | C    |
| 53  | 3     | 1383 | C    |
| 53  | 3     | 1384 | C    |
| 53  | 3     | 1394 | A    |
| 53  | 3     | 1397 | C    |
| 53  | 3     | 1399 | C    |
| 53  | 3     | 1446 | A    |
| 53  | 3     | 1448 | C    |
| 53  | 3     | 1452 | C    |
| 53  | 3     | 1492 | A    |
| 53  | 3     | 1494 | G    |
| 53  | 3     | 1502 | A    |
| 53  | 3     | 1503 | A    |
| 53  | 3     | 1505 | G    |
| 53  | 3     | 1506 | U    |
| 53  | 3     | 1517 | G    |
| 53  | 3     | 1529 | G    |
| 53  | 3     | 1530 | G    |
| 53  | 3     | 1534 | A    |
| 53  | 3     | 1535 | C    |
| 53  | 3     | 1540 | U    |
| 54  | 1     | 10   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | 1     | 12  | U    |
| 54  | 1     | 34  | U    |
| 54  | 1     | 35  | G    |
| 54  | 1     | 46  | G    |
| 54  | 1     | 50  | U    |
| 54  | 1     | 51  | G    |
| 54  | 1     | 63  | A    |
| 54  | 1     | 71  | A    |
| 54  | 1     | 74  | A    |
| 54  | 1     | 75  | G    |
| 54  | 1     | 103 | A    |
| 54  | 1     | 119 | A    |
| 54  | 1     | 120 | U    |
| 54  | 1     | 139 | U    |
| 54  | 1     | 140 | C    |
| 54  | 1     | 141 | G    |
| 54  | 1     | 142 | A    |
| 54  | 1     | 162 | U    |
| 54  | 1     | 163 | C    |
| 54  | 1     | 196 | A    |
| 54  | 1     | 216 | A    |
| 54  | 1     | 221 | A    |
| 54  | 1     | 222 | A    |
| 54  | 1     | 224 | U    |
| 54  | 1     | 228 | C    |
| 54  | 1     | 248 | G    |
| 54  | 1     | 249 | C    |
| 54  | 1     | 255 | A    |
| 54  | 1     | 266 | G    |
| 54  | 1     | 276 | U    |
| 54  | 1     | 281 | C    |
| 54  | 1     | 294 | A    |
| 54  | 1     | 301 | G    |
| 54  | 1     | 311 | A    |
| 54  | 1     | 323 | C    |
| 54  | 1     | 324 | A    |
| 54  | 1     | 329 | G    |
| 54  | 1     | 330 | A    |
| 54  | 1     | 353 | C    |
| 54  | 1     | 361 | G    |
| 54  | 1     | 371 | A    |
| 54  | 1     | 372 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | 1     | 386 | G    |
| 54  | 1     | 387 | U    |
| 54  | 1     | 404 | A    |
| 54  | 1     | 406 | G    |
| 54  | 1     | 411 | G    |
| 54  | 1     | 422 | A    |
| 54  | 1     | 424 | G    |
| 54  | 1     | 457 | A    |
| 54  | 1     | 481 | G    |
| 54  | 1     | 491 | G    |
| 54  | 1     | 504 | A    |
| 54  | 1     | 505 | A    |
| 54  | 1     | 518 | G    |
| 54  | 1     | 529 | A    |
| 54  | 1     | 530 | G    |
| 54  | 1     | 531 | C    |
| 54  | 1     | 532 | A    |
| 54  | 1     | 542 | C    |
| 54  | 1     | 543 | G    |
| 54  | 1     | 545 | U    |
| 54  | 1     | 547 | A    |
| 54  | 1     | 563 | A    |
| 54  | 1     | 573 | U    |
| 54  | 1     | 574 | A    |
| 54  | 1     | 603 | A    |
| 54  | 1     | 614 | A    |
| 54  | 1     | 616 | A    |
| 54  | 1     | 627 | A    |
| 54  | 1     | 637 | A    |
| 54  | 1     | 645 | C    |
| 54  | 1     | 646 | U    |
| 54  | 1     | 654 | A    |
| 54  | 1     | 669 | G    |
| 54  | 1     | 686 | U    |
| 54  | 1     | 687 | C    |
| 54  | 1     | 694 | U    |
| 54  | 1     | 695 | G    |
| 54  | 1     | 730 | A    |
| 54  | 1     | 747 | C    |
| 54  | 1     | 752 | A    |
| 54  | 1     | 764 | A    |
| 54  | 1     | 775 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | 1     | 776  | G    |
| 54  | 1     | 782  | A    |
| 54  | 1     | 784  | G    |
| 54  | 1     | 785  | G    |
| 54  | 1     | 805  | G    |
| 54  | 1     | 806  | C    |
| 54  | 1     | 812  | C    |
| 54  | 1     | 819  | A    |
| 54  | 1     | 827  | U    |
| 54  | 1     | 828  | U    |
| 54  | 1     | 830  | G    |
| 54  | 1     | 845  | A    |
| 54  | 1     | 846  | U    |
| 54  | 1     | 847  | U    |
| 54  | 1     | 858  | G    |
| 54  | 1     | 859  | G    |
| 54  | 1     | 860  | U    |
| 54  | 1     | 878  | A    |
| 54  | 1     | 885  | C    |
| 54  | 1     | 886  | A    |
| 54  | 1     | 887  | U    |
| 54  | 1     | 896  | A    |
| 54  | 1     | 897  | C    |
| 54  | 1     | 910  | A    |
| 54  | 1     | 932  | U    |
| 54  | 1     | 941  | A    |
| 54  | 1     | 946  | C    |
| 54  | 1     | 961  | C    |
| 54  | 1     | 962  | G    |
| 54  | 1     | 974  | G    |
| 54  | 1     | 983  | A    |
| 54  | 1     | 995  | C    |
| 54  | 1     | 996  | A    |
| 54  | 1     | 1012 | U    |
| 54  | 1     | 1013 | C    |
| 54  | 1     | 1021 | A    |
| 54  | 1     | 1022 | G    |
| 54  | 1     | 1033 | U    |
| 54  | 1     | 1045 | C    |
| 54  | 1     | 1046 | A    |
| 54  | 1     | 1054 | A    |
| 54  | 1     | 1056 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | 1     | 1062 | G    |
| 54  | 1     | 1063 | G    |
| 54  | 1     | 1064 | C    |
| 54  | 1     | 1065 | U    |
| 54  | 1     | 1066 | U    |
| 54  | 1     | 1067 | A    |
| 54  | 1     | 1068 | G    |
| 54  | 1     | 1070 | A    |
| 54  | 1     | 1071 | G    |
| 54  | 1     | 1076 | C    |
| 54  | 1     | 1079 | C    |
| 54  | 1     | 1082 | U    |
| 54  | 1     | 1084 | A    |
| 54  | 1     | 1085 | A    |
| 54  | 1     | 1088 | A    |
| 54  | 1     | 1104 | C    |
| 54  | 1     | 1106 | G    |
| 54  | 1     | 1111 | A    |
| 54  | 1     | 1131 | G    |
| 54  | 1     | 1132 | U    |
| 54  | 1     | 1135 | C    |
| 54  | 1     | 1143 | A    |
| 54  | 1     | 1157 | G    |
| 54  | 1     | 1175 | A    |
| 54  | 1     | 1176 | U    |
| 54  | 1     | 1177 | G    |
| 54  | 1     | 1180 | U    |
| 54  | 1     | 1181 | U    |
| 54  | 1     | 1212 | G    |
| 54  | 1     | 1251 | C    |
| 54  | 1     | 1253 | A    |
| 54  | 1     | 1256 | G    |
| 54  | 1     | 1271 | G    |
| 54  | 1     | 1272 | A    |
| 54  | 1     | 1301 | A    |
| 54  | 1     | 1321 | A    |
| 54  | 1     | 1329 | U    |
| 54  | 1     | 1330 | C    |
| 54  | 1     | 1345 | C    |
| 54  | 1     | 1365 | A    |
| 54  | 1     | 1378 | A    |
| 54  | 1     | 1379 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | 1     | 1383 | A    |
| 54  | 1     | 1395 | A    |
| 54  | 1     | 1398 | C    |
| 54  | 1     | 1416 | G    |
| 54  | 1     | 1419 | A    |
| 54  | 1     | 1420 | A    |
| 54  | 1     | 1428 | C    |
| 54  | 1     | 1454 | C    |
| 54  | 1     | 1461 | C    |
| 54  | 1     | 1476 | U    |
| 54  | 1     | 1482 | G    |
| 54  | 1     | 1490 | A    |
| 54  | 1     | 1498 | C    |
| 54  | 1     | 1504 | A    |
| 54  | 1     | 1515 | A    |
| 54  | 1     | 1524 | G    |
| 54  | 1     | 1533 | C    |
| 54  | 1     | 1535 | A    |
| 54  | 1     | 1536 | C    |
| 54  | 1     | 1537 | G    |
| 54  | 1     | 1555 | G    |
| 54  | 1     | 1559 | U    |
| 54  | 1     | 1560 | G    |
| 54  | 1     | 1565 | C    |
| 54  | 1     | 1569 | A    |
| 54  | 1     | 1578 | U    |
| 54  | 1     | 1581 | G    |
| 54  | 1     | 1584 | U    |
| 54  | 1     | 1585 | C    |
| 54  | 1     | 1608 | A    |
| 54  | 1     | 1611 | C    |
| 54  | 1     | 1616 | A    |
| 54  | 1     | 1647 | U    |
| 54  | 1     | 1648 | U    |
| 54  | 1     | 1654 | A    |
| 54  | 1     | 1674 | G    |
| 54  | 1     | 1703 | G    |
| 54  | 1     | 1715 | G    |
| 54  | 1     | 1729 | U    |
| 54  | 1     | 1730 | C    |
| 54  | 1     | 1738 | G    |
| 54  | 1     | 1758 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | 1     | 1764 | C    |
| 54  | 1     | 1773 | A    |
| 54  | 1     | 1780 | A    |
| 54  | 1     | 1791 | A    |
| 54  | 1     | 1800 | C    |
| 54  | 1     | 1801 | A    |
| 54  | 1     | 1808 | A    |
| 54  | 1     | 1816 | C    |
| 54  | 1     | 1829 | A    |
| 54  | 1     | 1871 | A    |
| 54  | 1     | 1901 | A    |
| 54  | 1     | 1906 | G    |
| 54  | 1     | 1907 | G    |
| 54  | 1     | 1913 | A    |
| 54  | 1     | 1929 | G    |
| 54  | 1     | 1930 | G    |
| 54  | 1     | 1937 | A    |
| 54  | 1     | 1938 | A    |
| 54  | 1     | 1944 | U    |
| 54  | 1     | 1955 | U    |
| 54  | 1     | 1962 | C    |
| 54  | 1     | 1963 | U    |
| 54  | 1     | 1967 | C    |
| 54  | 1     | 1970 | A    |
| 54  | 1     | 1971 | U    |
| 54  | 1     | 1972 | G    |
| 54  | 1     | 1991 | U    |
| 54  | 1     | 1997 | C    |
| 54  | 1     | 2020 | A    |
| 54  | 1     | 2022 | U    |
| 54  | 1     | 2023 | C    |
| 54  | 1     | 2030 | A    |
| 54  | 1     | 2031 | A    |
| 54  | 1     | 2043 | C    |
| 54  | 1     | 2049 | G    |
| 54  | 1     | 2052 | A    |
| 54  | 1     | 2055 | C    |
| 54  | 1     | 2056 | G    |
| 54  | 1     | 2060 | A    |
| 54  | 1     | 2061 | G    |
| 54  | 1     | 2062 | A    |
| 54  | 1     | 2069 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | 1     | 2072 | C    |
| 54  | 1     | 2096 | C    |
| 54  | 1     | 2098 | U    |
| 54  | 1     | 2110 | G    |
| 54  | 1     | 2111 | U    |
| 54  | 1     | 2112 | G    |
| 54  | 1     | 2113 | U    |
| 54  | 1     | 2115 | G    |
| 54  | 1     | 2118 | U    |
| 54  | 1     | 2119 | A    |
| 54  | 1     | 2125 | G    |
| 54  | 1     | 2129 | C    |
| 54  | 1     | 2131 | U    |
| 54  | 1     | 2132 | U    |
| 54  | 1     | 2133 | G    |
| 54  | 1     | 2145 | C    |
| 54  | 1     | 2147 | A    |
| 54  | 1     | 2162 | G    |
| 54  | 1     | 2172 | U    |
| 54  | 1     | 2173 | A    |
| 54  | 1     | 2174 | C    |
| 54  | 1     | 2176 | A    |
| 54  | 1     | 2189 | U    |
| 54  | 1     | 2198 | A    |
| 54  | 1     | 2203 | U    |
| 54  | 1     | 2204 | G    |
| 54  | 1     | 2211 | A    |
| 54  | 1     | 2212 | A    |
| 54  | 1     | 2213 | U    |
| 54  | 1     | 2225 | A    |
| 54  | 1     | 2239 | G    |
| 54  | 1     | 2268 | A    |
| 54  | 1     | 2278 | A    |
| 54  | 1     | 2283 | C    |
| 54  | 1     | 2287 | A    |
| 54  | 1     | 2297 | A    |
| 54  | 1     | 2305 | U    |
| 54  | 1     | 2309 | A    |
| 54  | 1     | 2325 | G    |
| 54  | 1     | 2327 | A    |
| 54  | 1     | 2334 | U    |
| 54  | 1     | 2337 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | 1     | 2345 | G    |
| 54  | 1     | 2350 | C    |
| 54  | 1     | 2383 | G    |
| 54  | 1     | 2385 | C    |
| 54  | 1     | 2392 | A    |
| 54  | 1     | 2402 | U    |
| 54  | 1     | 2406 | A    |
| 54  | 1     | 2423 | U    |
| 54  | 1     | 2424 | C    |
| 54  | 1     | 2425 | A    |
| 54  | 1     | 2426 | A    |
| 54  | 1     | 2427 | C    |
| 54  | 1     | 2429 | G    |
| 54  | 1     | 2430 | A    |
| 54  | 1     | 2435 | A    |
| 54  | 1     | 2441 | U    |
| 54  | 1     | 2448 | A    |
| 54  | 1     | 2476 | A    |
| 54  | 1     | 2494 | G    |
| 54  | 1     | 2498 | C    |
| 54  | 1     | 2502 | G    |
| 54  | 1     | 2505 | G    |
| 54  | 1     | 2518 | A    |
| 54  | 1     | 2529 | G    |
| 54  | 1     | 2547 | A    |
| 54  | 1     | 2554 | U    |
| 54  | 1     | 2566 | A    |
| 54  | 1     | 2567 | G    |
| 54  | 1     | 2572 | A    |
| 54  | 1     | 2602 | A    |
| 54  | 1     | 2603 | G    |
| 54  | 1     | 2609 | U    |
| 54  | 1     | 2613 | U    |
| 54  | 1     | 2629 | U    |
| 54  | 1     | 2646 | C    |
| 54  | 1     | 2655 | G    |
| 54  | 1     | 2682 | A    |
| 54  | 1     | 2689 | U    |
| 54  | 1     | 2690 | U    |
| 54  | 1     | 2714 | G    |
| 54  | 1     | 2716 | C    |
| 54  | 1     | 2744 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | 1     | 2748 | A    |
| 54  | 1     | 2757 | A    |
| 54  | 1     | 2764 | A    |
| 54  | 1     | 2765 | A    |
| 54  | 1     | 2778 | A    |
| 54  | 1     | 2779 | U    |
| 54  | 1     | 2791 | G    |
| 54  | 1     | 2794 | C    |
| 54  | 1     | 2797 | U    |
| 54  | 1     | 2800 | A    |
| 54  | 1     | 2801 | G    |
| 54  | 1     | 2809 | A    |
| 54  | 1     | 2820 | A    |
| 54  | 1     | 2821 | A    |
| 54  | 1     | 2833 | U    |
| 54  | 1     | 2867 | G    |
| 54  | 1     | 2868 | A    |
| 54  | 1     | 2872 | A    |
| 54  | 1     | 2880 | C    |
| 54  | 1     | 2883 | A    |
| 54  | 1     | 2884 | U    |
| 55  | 2     | 4    | C    |
| 55  | 2     | 13   | G    |
| 55  | 2     | 24   | G    |
| 55  | 2     | 35   | C    |
| 55  | 2     | 40   | U    |
| 55  | 2     | 44   | G    |
| 55  | 2     | 51   | G    |
| 55  | 2     | 67   | G    |
| 55  | 2     | 89   | U    |
| 55  | 2     | 90   | C    |
| 55  | 2     | 108  | A    |
| 55  | 2     | 109  | A    |
| 56  | 5     | 3    | G    |
| 56  | 5     | 4    | C    |
| 56  | 5     | 5    | G    |
| 56  | 5     | 6    | A    |
| 56  | 5     | 9    | A    |
| 56  | 5     | 14   | A    |
| 56  | 5     | 18   | G    |
| 56  | 5     | 19   | G    |
| 56  | 5     | 20   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | 5     | 21  | A    |
| 56  | 5     | 42  | G    |
| 56  | 5     | 47  | U    |
| 56  | 5     | 48  | C    |
| 56  | 5     | 61  | C    |
| 56  | 5     | 73  | A    |
| 56  | 5     | 76  | A    |
| 57  | 6     | 2   | G    |
| 57  | 6     | 3   | C    |
| 57  | 6     | 8   | U    |
| 57  | 6     | 9   | G    |
| 57  | 6     | 10  | G    |
| 57  | 6     | 14  | A    |
| 57  | 6     | 17  | C    |
| 57  | 6     | 19  | G    |
| 57  | 6     | 20  | U    |
| 57  | 6     | 21  | A    |
| 57  | 6     | 22  | G    |
| 57  | 6     | 28  | C    |
| 57  | 6     | 33  | U    |
| 57  | 6     | 34  | C    |
| 57  | 6     | 35  | A    |
| 57  | 6     | 39  | C    |
| 57  | 6     | 46  | G    |
| 57  | 6     | 61  | C    |
| 57  | 6     | 64  | G    |
| 57  | 6     | 65  | C    |
| 57  | 6     | 69  | C    |
| 57  | 6     | 70  | G    |
| 57  | 6     | 76  | A    |
| 58  | 4     | 16  | A    |
| 58  | 4     | 20  | C    |
| 58  | 4     | 21  | C    |

All (36) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 3     | 70  | U    |
| 53  | 3     | 280 | C    |
| 53  | 3     | 328 | C    |
| 53  | 3     | 413 | G    |
| 53  | 3     | 438 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 3     | 928  | G    |
| 53  | 3     | 965  | U    |
| 53  | 3     | 1061 | G    |
| 53  | 3     | 1078 | U    |
| 53  | 3     | 1164 | G    |
| 53  | 3     | 1168 | U    |
| 53  | 3     | 1183 | U    |
| 53  | 3     | 1201 | A    |
| 53  | 3     | 1280 | A    |
| 53  | 3     | 1305 | G    |
| 53  | 3     | 1347 | G    |
| 53  | 3     | 1493 | A    |
| 54  | 1     | 227  | A    |
| 54  | 1     | 421  | C    |
| 54  | 1     | 490  | C    |
| 54  | 1     | 774  | G    |
| 54  | 1     | 859  | G    |
| 54  | 1     | 1020 | A    |
| 54  | 1     | 1130 | U    |
| 54  | 1     | 1475 | G    |
| 54  | 1     | 2286 | G    |
| 54  | 1     | 2296 | U    |
| 54  | 1     | 2326 | C    |
| 54  | 1     | 2333 | A    |
| 54  | 1     | 2391 | G    |
| 54  | 1     | 2756 | U    |
| 54  | 1     | 2808 | G    |
| 55  | 2     | 66   | A    |
| 55  | 2     | 88   | C    |
| 56  | 5     | 2    | G    |
| 56  | 5     | 3    | G    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 62  | GCP  | 8     | 801  | 63    | 32,34,34     | 2.56 | 6 (18%)  | 49,54,54    | 2.52 | 15 (30%) |
| 61  | PRO  | 5     | 101  | 56,60 | 6,7,8        | 0.57 | 0        | 7,8,10      | 1.23 | 1 (14%)  |
| 60  | FME  | 1     | 3001 | 61    | 8,9,10       | 0.73 | 0        | 8,9,11      | 1.13 | 1 (12%)  |

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

| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 62  | GCP  | 8     | 801  | 63    | -       | 9/19/38/38 | 0/3/3/3 |
| 61  | PRO  | 5     | 101  | 56,60 | -       | 0/0/9/11   | 0/1/1/1 |
| 60  | FME  | 1     | 3001 | 61    | -       | 1/7/9/11   | -       |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 62  | 8     | 801 | GCP  | PA-O3A | -9.79 | 1.48        | 1.59     |
| 62  | 8     | 801 | GCP  | PB-O3A | -8.23 | 1.49        | 1.58     |
| 62  | 8     | 801 | GCP  | PB-O2B | -2.93 | 1.49        | 1.56     |
| 62  | 8     | 801 | GCP  | PG-O2G | -2.59 | 1.49        | 1.55     |
| 62  | 8     | 801 | GCP  | PG-O3G | -2.52 | 1.49        | 1.55     |
| 62  | 8     | 801 | GCP  | C1'-N9 | 2.23  | 1.53        | 1.47     |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 62  | 8     | 801 | GCP  | C1'-N9-C4  | 8.24  | 150.81      | 126.49   |
| 62  | 8     | 801 | GCP  | C1'-N9-C8  | -8.19 | 103.47      | 126.73   |
| 62  | 8     | 801 | GCP  | O3A-PA-O1A | -4.56 | 96.97       | 110.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 62  | 8     | 801  | GCP  | O2G-PG-C3B  | -4.47 | 95.54       | 106.40   |
| 62  | 8     | 801  | GCP  | O3G-PG-O2G  | 4.28  | 120.16      | 107.96   |
| 62  | 8     | 801  | GCP  | O2B-PB-O1B  | 3.84  | 122.45      | 109.95   |
| 62  | 8     | 801  | GCP  | O3'-C3'-C4' | -3.52 | 100.98      | 111.08   |
| 62  | 8     | 801  | GCP  | O4'-C1'-C2' | -2.93 | 100.35      | 106.62   |
| 62  | 8     | 801  | GCP  | O1B-PB-C3B  | 2.86  | 116.58      | 109.05   |
| 62  | 8     | 801  | GCP  | PB-O3A-PA   | 2.80  | 141.52      | 132.37   |
| 62  | 8     | 801  | GCP  | O2A-PA-O5'  | -2.73 | 95.19       | 107.57   |
| 62  | 8     | 801  | GCP  | O3G-PG-O1G  | -2.55 | 105.80      | 112.39   |
| 62  | 8     | 801  | GCP  | O2A-PA-O3A  | 2.51  | 114.05      | 107.27   |
| 62  | 8     | 801  | GCP  | O4'-C4'-C5' | 2.38  | 116.95      | 109.33   |
| 62  | 8     | 801  | GCP  | O2A-PA-O1A  | 2.37  | 123.47      | 112.44   |
| 61  | 5     | 101  | PRO  | O-C-CA      | -2.24 | 119.01      | 124.77   |
| 60  | 1     | 3001 | FME  | CA-N-CN     | -2.23 | 119.39      | 122.82   |

There are no chirality outliers.

All (10) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 60  | 1     | 3001 | FME  | O1-CN-N-CA      |
| 62  | 8     | 801  | GCP  | PB-C3B-PG-O1G   |
| 62  | 8     | 801  | GCP  | PG-C3B-PB-O1B   |
| 62  | 8     | 801  | GCP  | C5'-O5'-PA-O1A  |
| 62  | 8     | 801  | GCP  | O4'-C4'-C5'-O5' |
| 62  | 8     | 801  | GCP  | PB-C3B-PG-O2G   |
| 62  | 8     | 801  | GCP  | PB-C3B-PG-O3G   |
| 62  | 8     | 801  | GCP  | C5'-O5'-PA-O3A  |
| 62  | 8     | 801  | GCP  | C5'-O5'-PA-O2A  |
| 62  | 8     | 801  | GCP  | C3'-C4'-C5'-O5' |

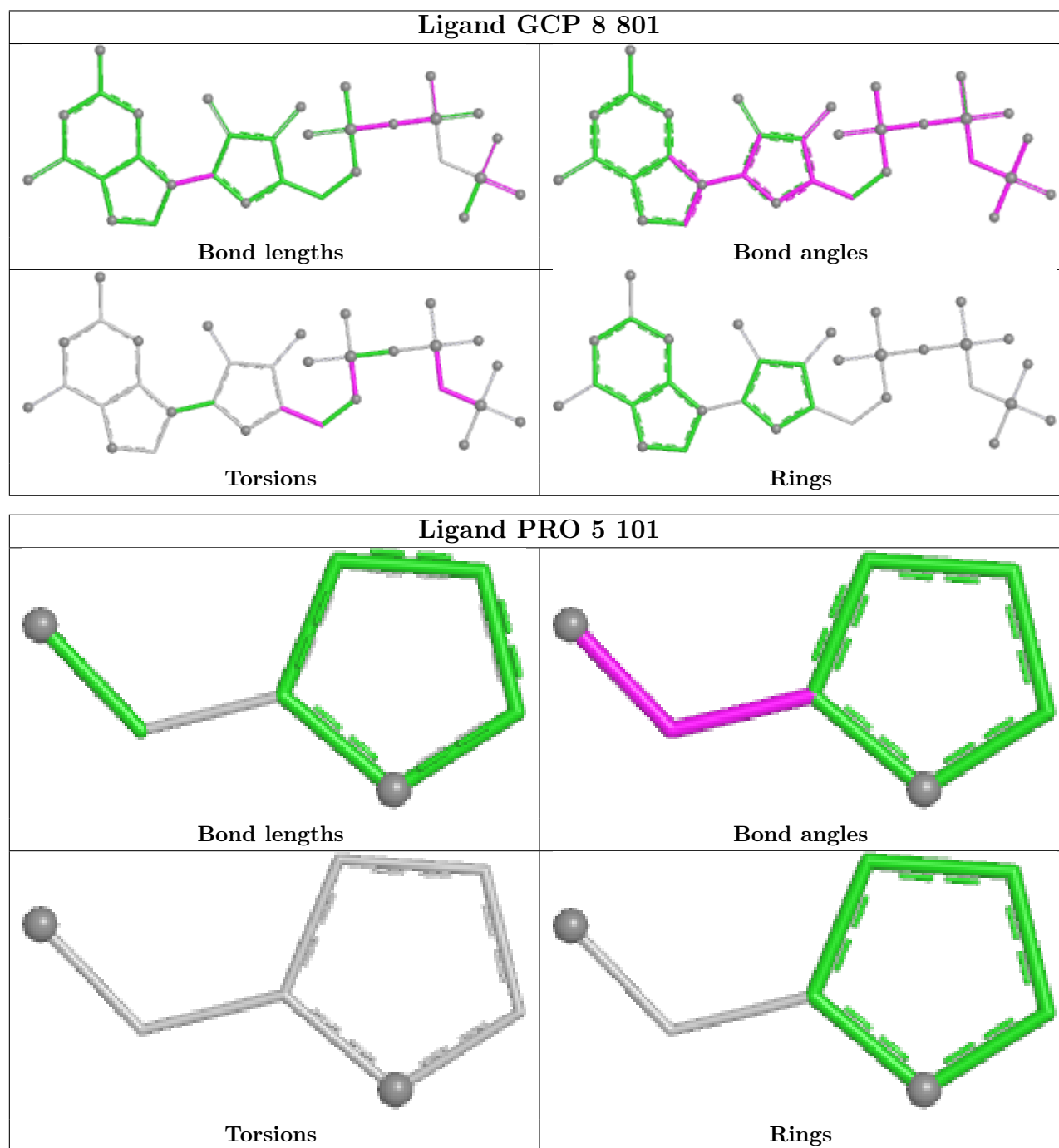
There are no ring outliers.

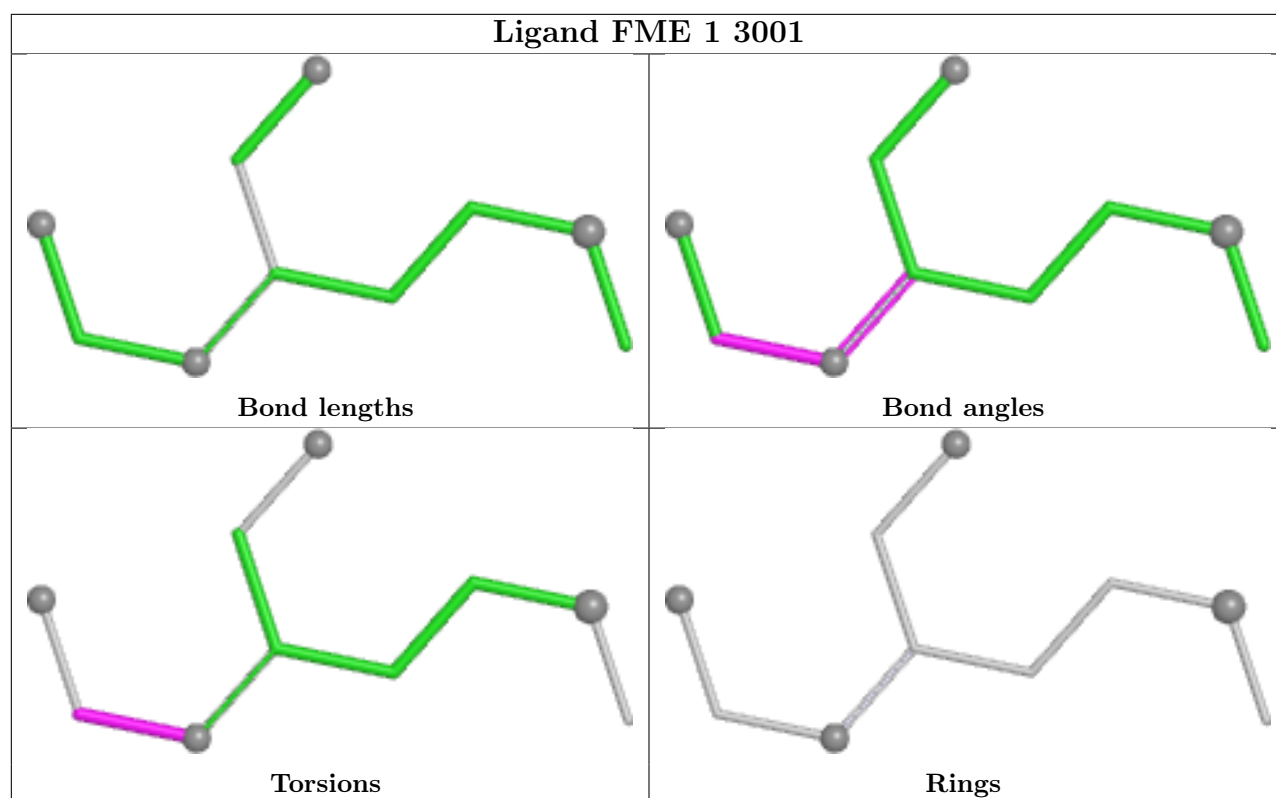
1 monomer is involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 62  | 8     | 801 | GCP  | 3       | 0            |

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.

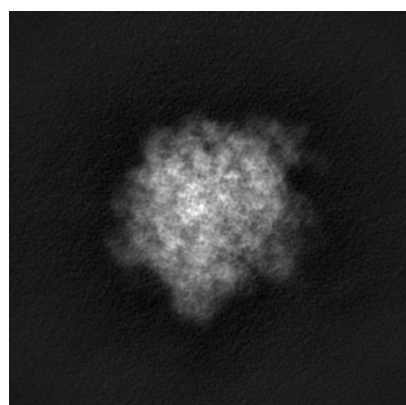
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22673. These allow visual inspection of the internal detail of the map and identification of artifacts.

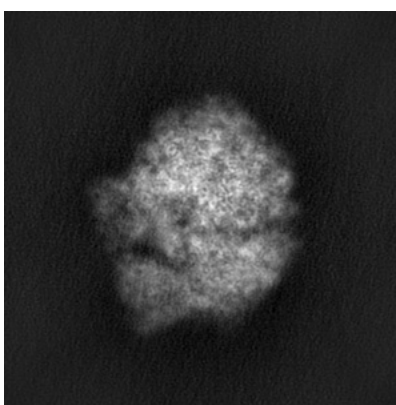
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

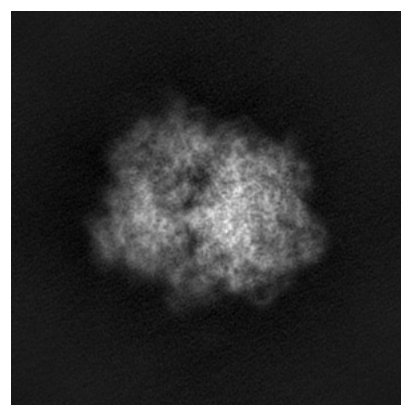
#### 6.1.1 Primary map



X



Y

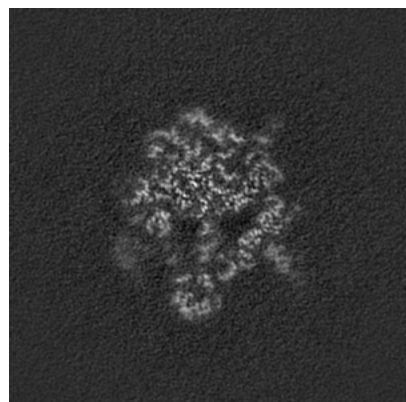


Z

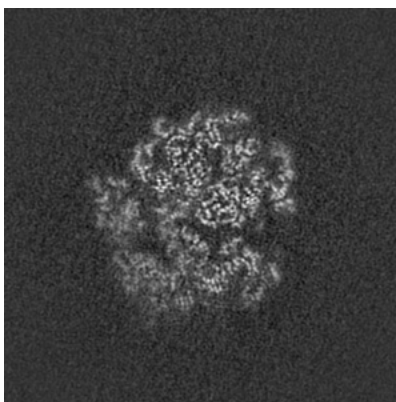
The images above show the map projected in three orthogonal directions.

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

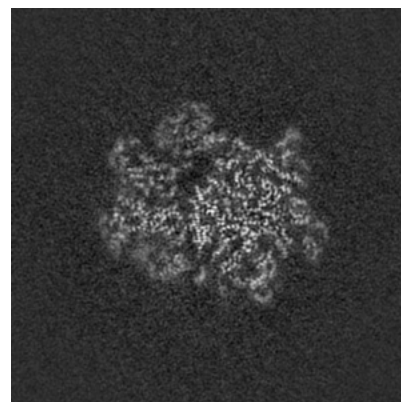
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

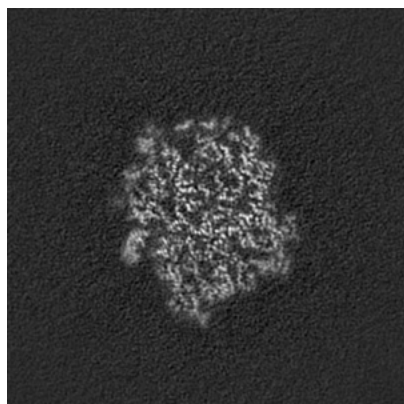


Z Index: 200

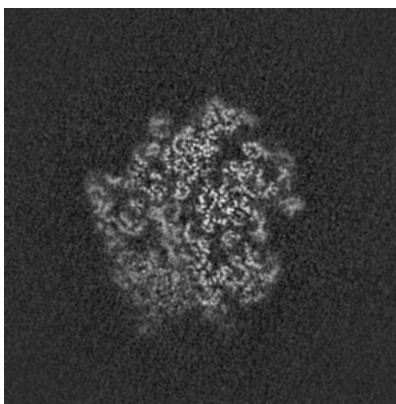
The images above show central slices of the map in three orthogonal directions.

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

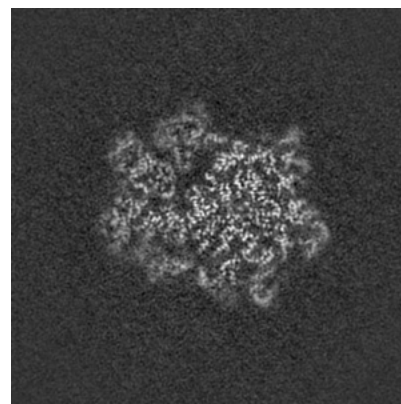
### 6.3.1 Primary map



X Index: 222



Y Index: 193

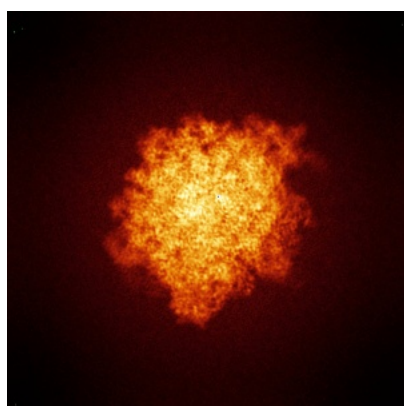


Z Index: 203

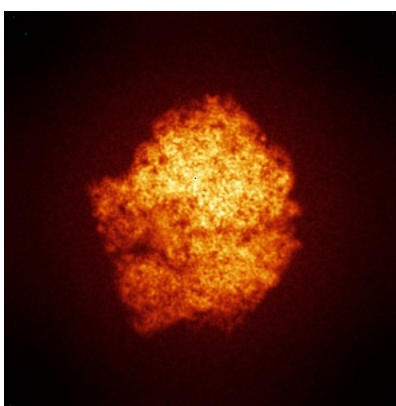
The images above show the largest variance slices of the map in three orthogonal directions.

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

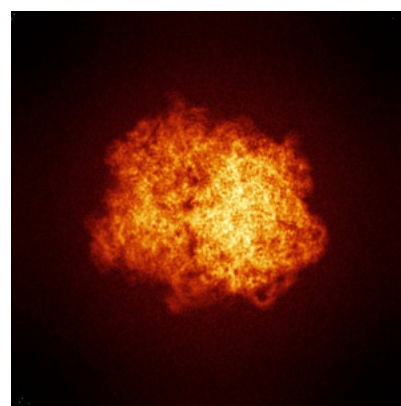
### 6.4.1 Primary map



X



Y



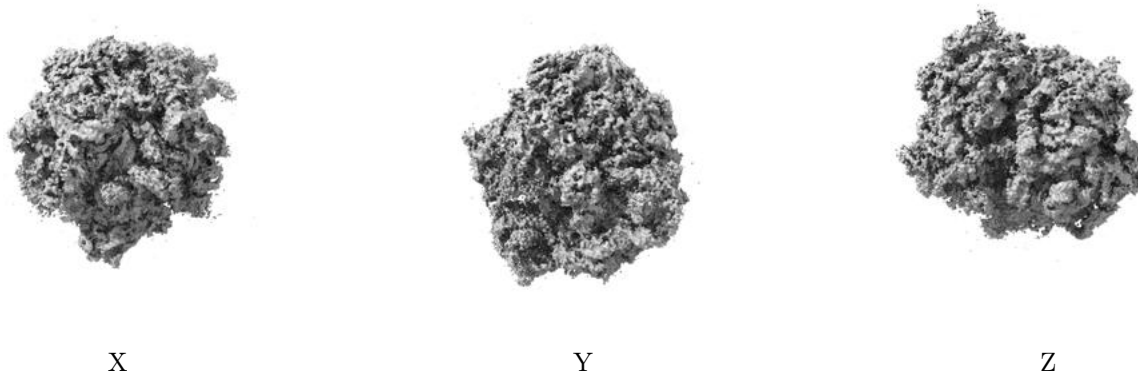
Z

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



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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

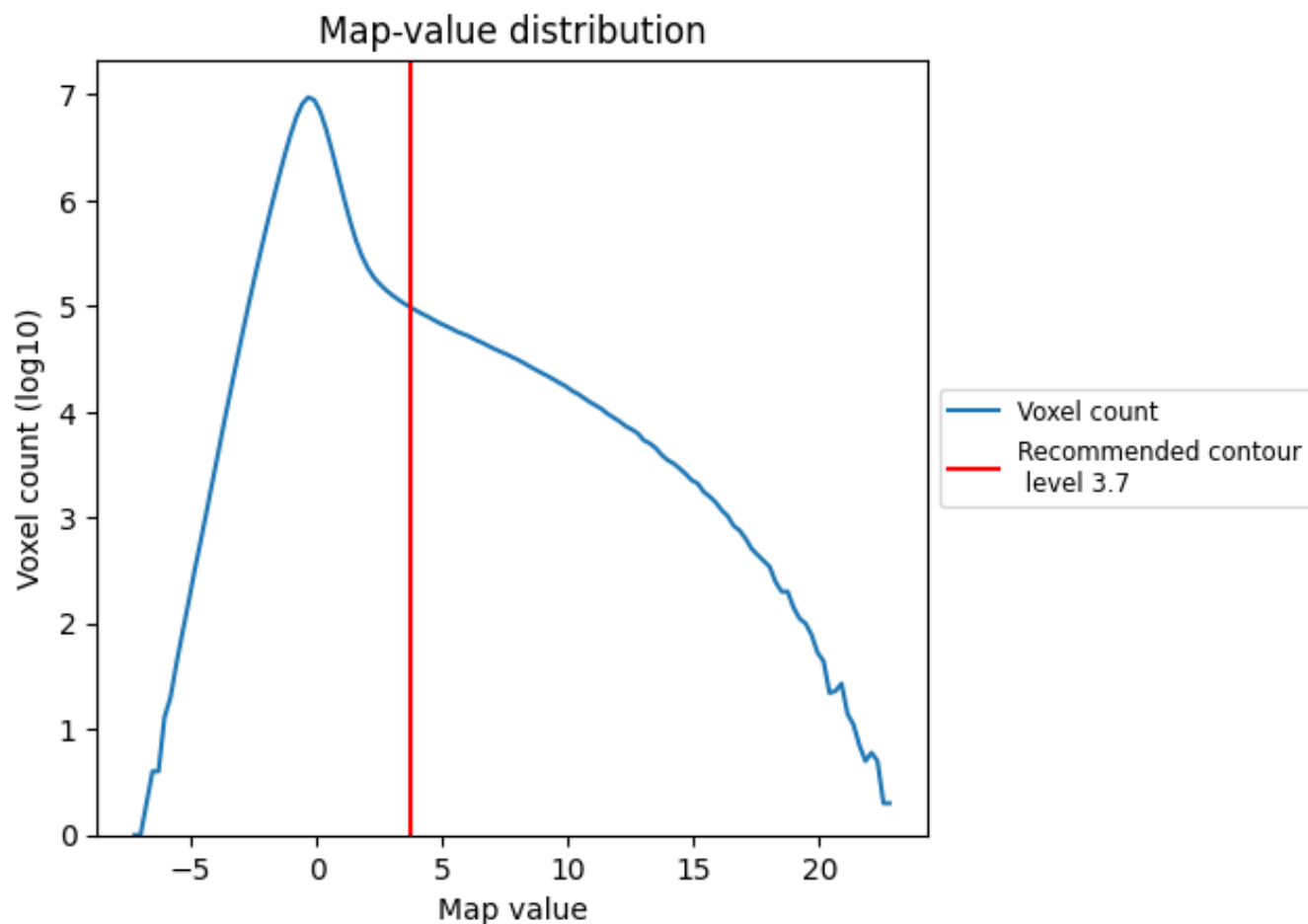
## 6.6 Mask visualisation [i](#)

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.

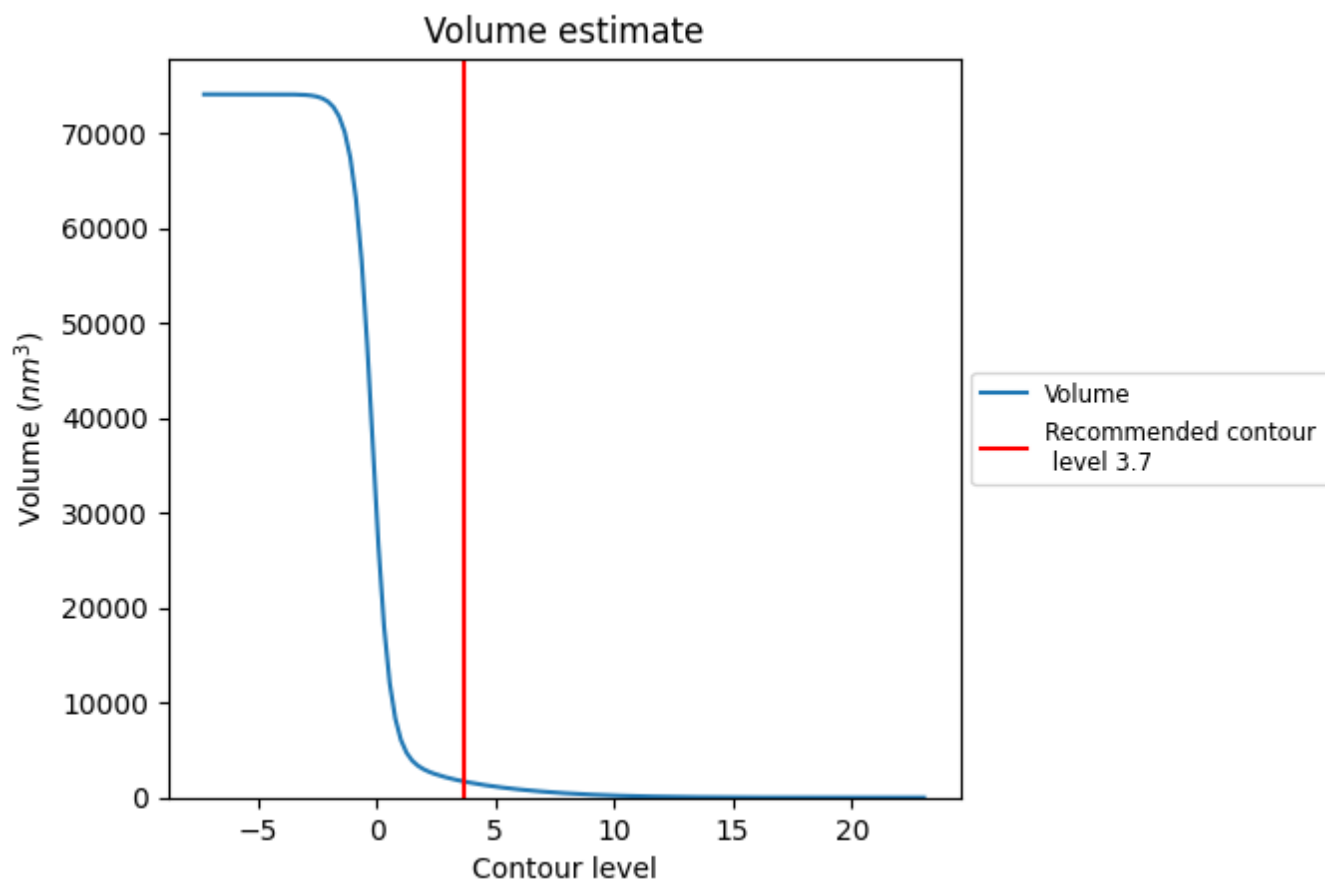
### 7.1 Map-value distribution [i](#)



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.



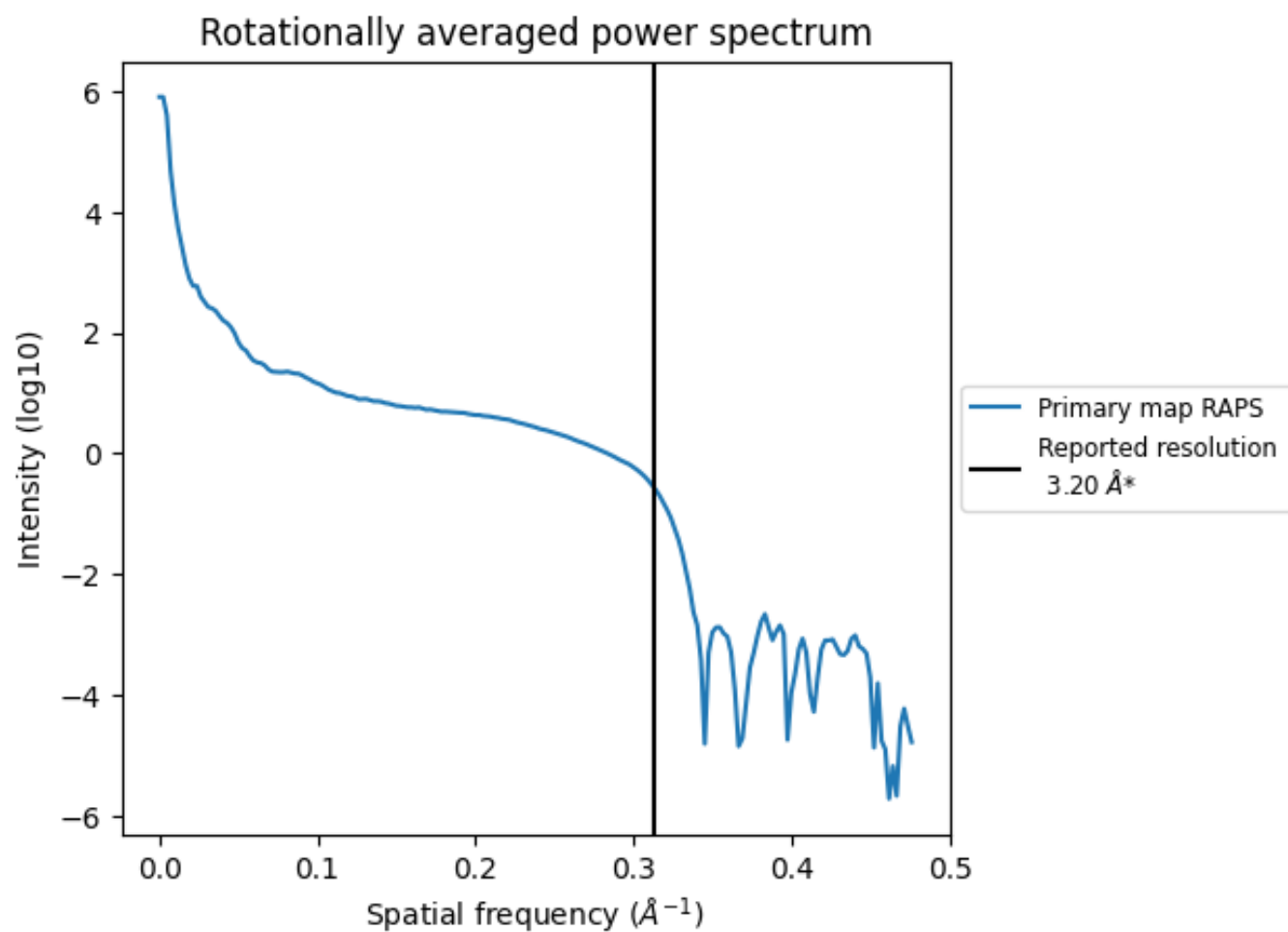
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1689 nm<sup>3</sup>; this corresponds to an approximate mass of 1525 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 0.312 Å<sup>-1</sup>

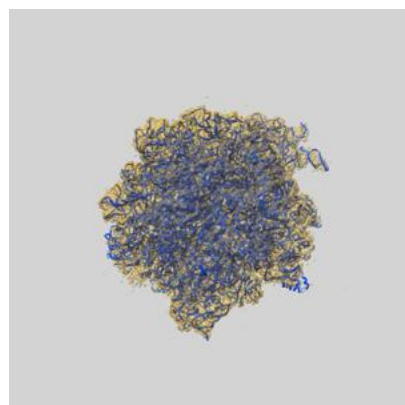
## 8 Fourier-Shell correlation

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

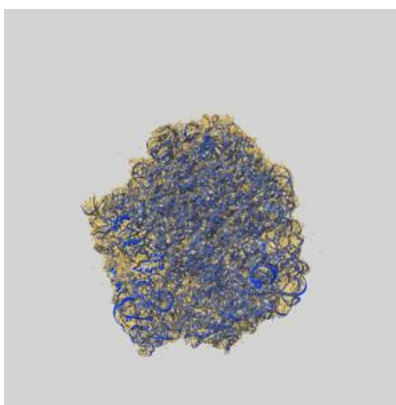
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22673 and PDB model 7K54. Per-residue inclusion information can be found in section [3](#) on page [17](#).

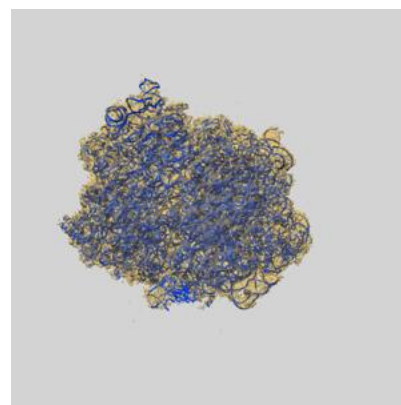
### 9.1 Map-model overlay [i](#)



X



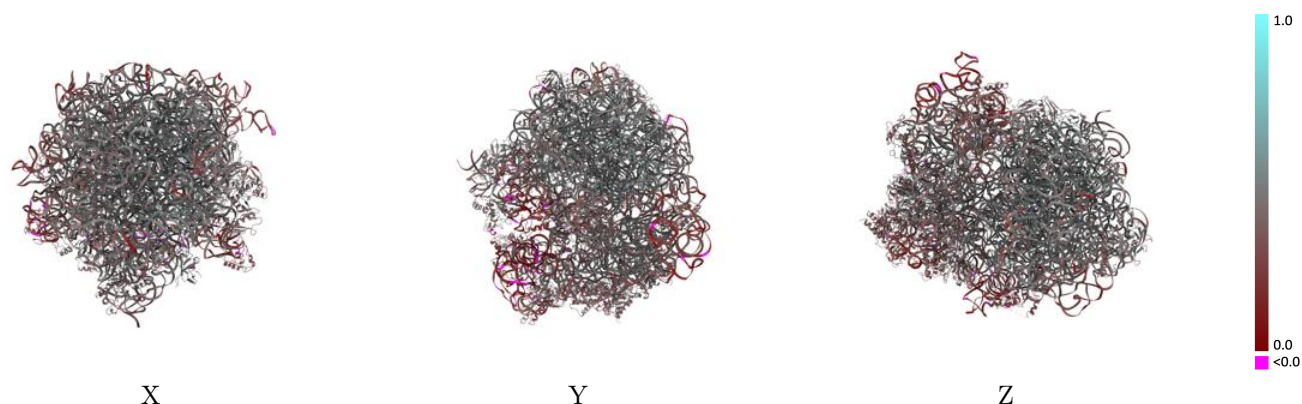
Y



Z

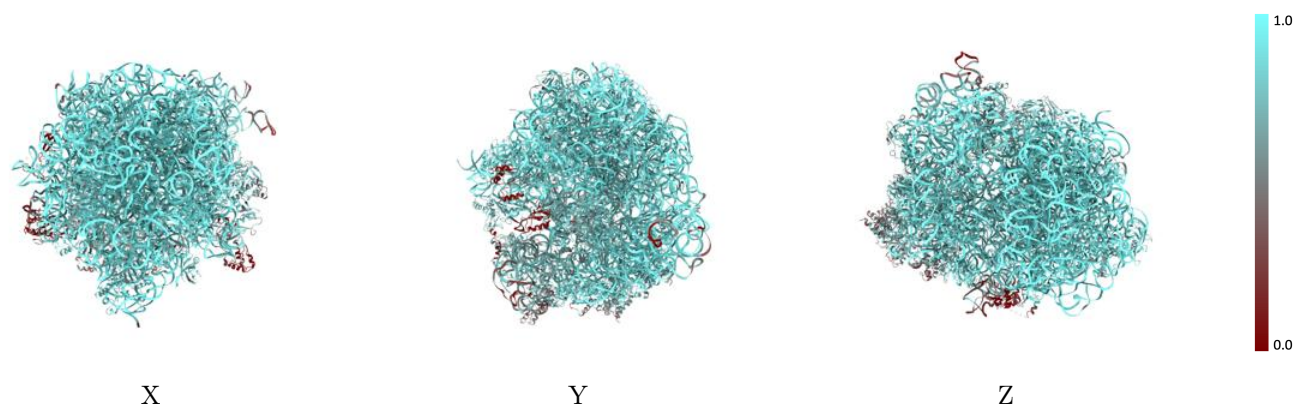
The images above show the 3D surface view of the map at the recommended contour level 3.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



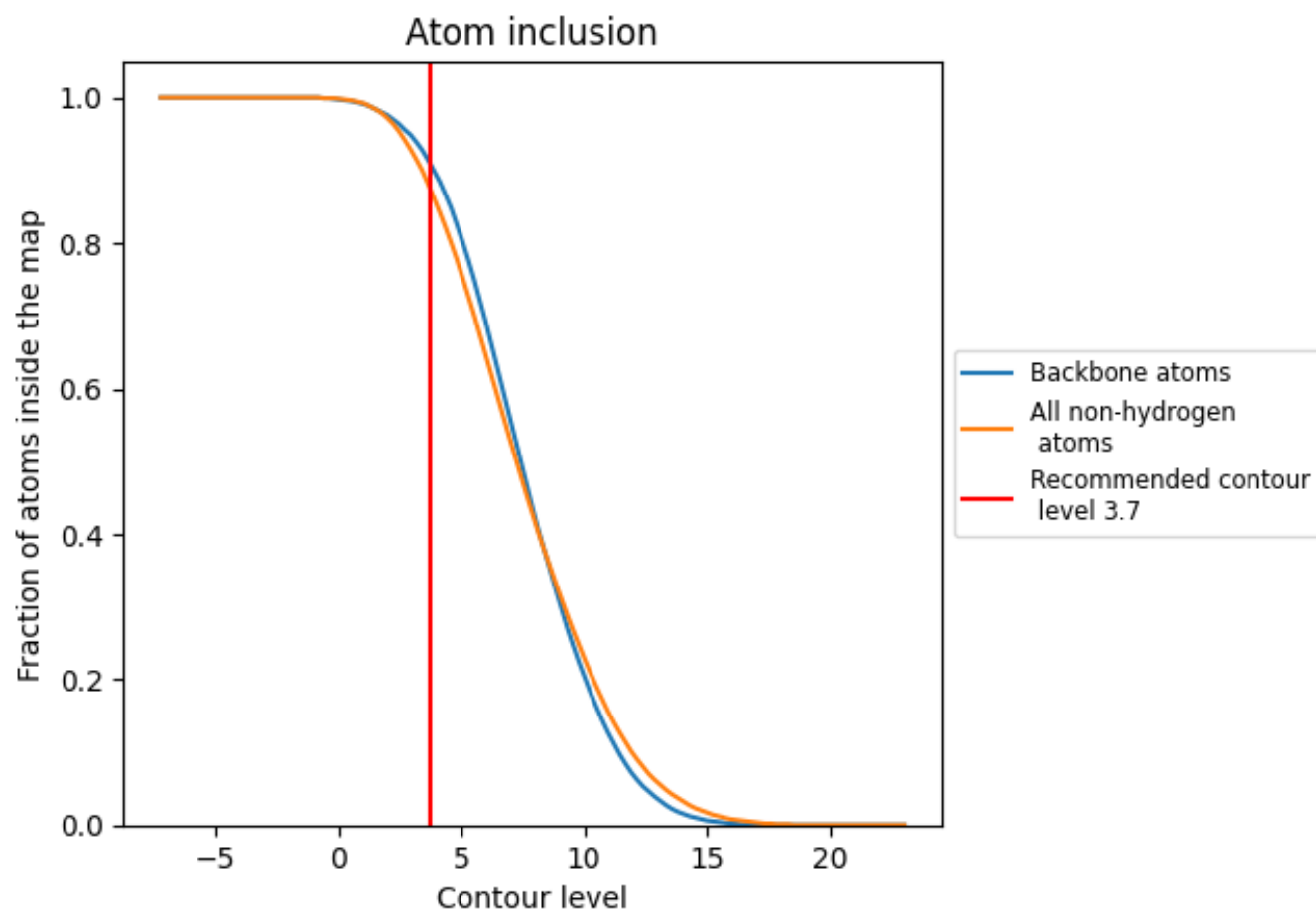
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.7).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 88% 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 (3.7) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8770   |  0.4060   |
| 1     |  0.9620   |  0.4380   |
| 2     |  0.9610   |  0.4100   |
| 3     |  0.8840   |  0.3450   |
| 4     |  0.7250   |  0.3410   |
| 5     |  0.9400   |  0.3580   |
| 6     |  0.9010   |  0.3430   |
| 8     |  0.7550   |  0.3830   |
| A     |  0.5940   |  0.2860   |
| B     |  0.9110   |  0.4640   |
| C     |  0.7090   |  0.4330   |
| D     |  0.9150   |  0.4900   |
| E     |  0.9270   |  0.4920   |
| F     |  0.9140   |  0.4770   |
| G     |  0.5410  |  0.3570  |
| H     |  0.6950 |  0.4040 |
| I     |  0.7600 |  0.3970 |
| J     |  0.8410 |  0.4310 |
| K     |  0.8280 |  0.3880 |
| L     |  0.4950 |  0.3060 |
| M     |  0.8410 |  0.4260 |
| N     |  0.6540 |  0.3620 |
| O     |  0.5310 |  0.3510 |
| P     |  0.8740 |  0.4050 |
| Q     |  0.8390 |  0.4580 |
| R     |  0.6050 |  0.3240 |
| S     |  0.7910 |  0.3810 |
| T     |  0.8510 |  0.4080 |
| U     |  0.8090 |  0.4220 |
| V     |  0.8640 |  0.4190 |
| W     |  0.8370 |  0.4010 |
| X     |  0.7640 |  0.3280 |
| Y     |  0.8260 |  0.3950 |
| Z     |  0.7320 |  0.3320 |
| a     |  0.2020 |  0.2340 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| b     |  0.9190   |  0.4940   |
| c     |  0.9000   |  0.4780   |
| d     |  0.7920   |  0.4420   |
| e     |  0.8110   |  0.3850   |
| f     |  0.8220   |  0.4250   |
| g     |  0.2380   |  0.3080   |
| h     |  0.1120   |  0.2330   |
| i     |  0.1320   |  0.2020   |
| j     |  0.9000   |  0.4660   |
| k     |  0.8810   |  0.4820   |
| l     |  0.8850   |  0.4720   |
| m     |  0.9110   |  0.4820   |
| n     |  0.9130   |  0.4690   |
| o     |  0.8620   |  0.4220   |
| p     |  0.8820   |  0.4710   |
| q     |  0.9140   |  0.4790   |
| r     |  0.8530   |  0.4650   |
| s     |  0.8770  |  0.4680  |
| t     |  0.8490 |  0.4550 |
| u     |  0.8310 |  0.4200 |
| v     |  0.8480 |  0.4540 |
| w     |  0.9070 |  0.4890 |
| x     |  0.9030 |  0.4690 |
| y     |  0.7540 |  0.3880 |
| z     |  0.8740 |  0.4560 |