



## Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:18 AM UTC

PDB ID : 6OGF / pdb\_00006ogf  
EMDB ID : EMD-20056  
Title : 70S termination complex with RF2 bound to the UGA codon. Partially rotated ribosome with RF2 bound (Structure III).  
Authors : Svidritskiy, E.; Demo, G.; Loveland, A.B.; Xu, C.; Korostelev, A.A.  
Deposited on : 2019-04-02  
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

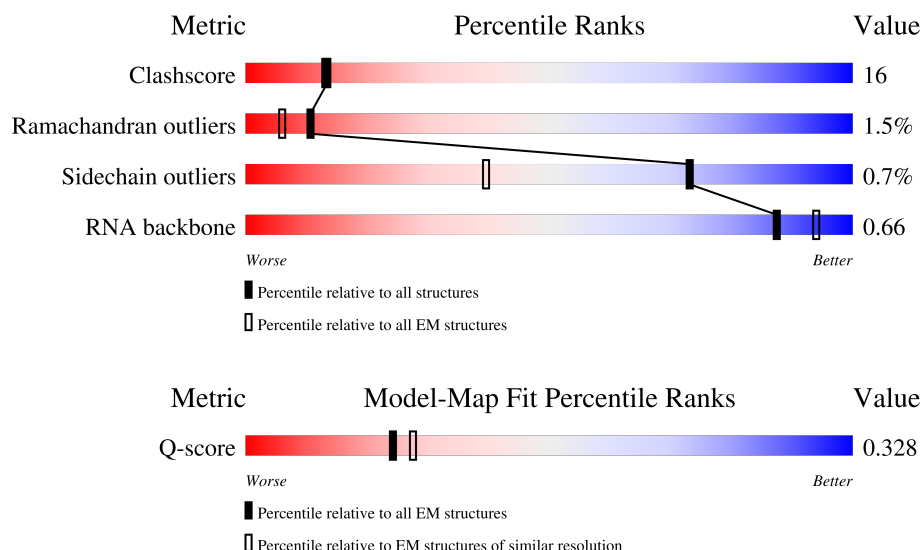
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 Å.

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



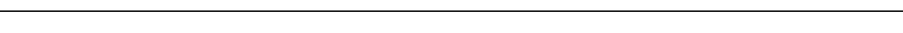
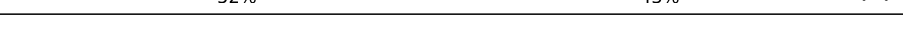
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 8855 ( 3.40 - 4.40 )                                     |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | b     | 273    |                  |
| 2   | c     | 209    |                  |
| 3   | d     | 201    |                  |

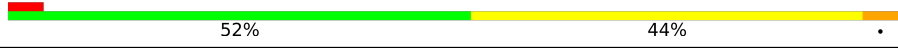
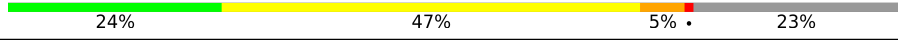
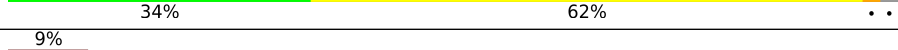
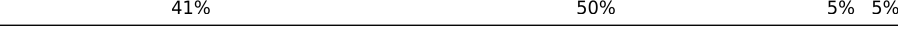
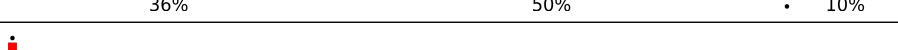
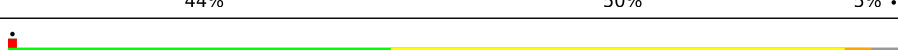
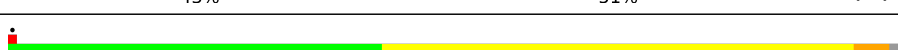
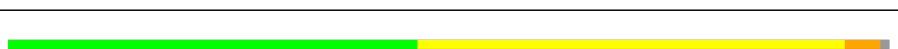
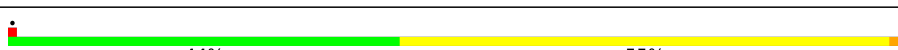
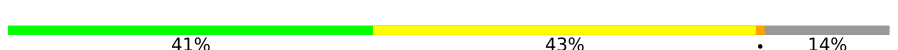
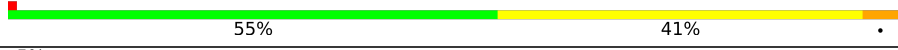
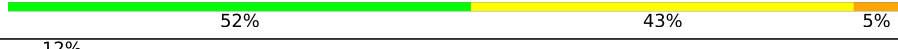
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| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 4   | e     | 179    |  42% 55% ..     |
| 5   | f     | 177    |  54% 44% ..     |
| 6   | g     | 149    |  56% 46% 50% 5% |
| 7   | j     | 142    |  62% 37% .      |
| 8   | k     | 123    |  63% 36% .      |
| 9   | l     | 144    |  70% 26% ..     |
| 10  | m     | 136    |  53% 44% .      |
| 11  | n     | 127    |  54% 39% . 6%   |
| 12  | o     | 117    |  55% 43% ...    |
| 13  | p     | 115    |  52% 43% ..     |
| 14  | q     | 118    |  57% 41% ..     |
| 15  | r     | 103    |  50% 47% .      |
| 16  | s     | 110    |  55% 45%      |
| 17  | t     | 100    |  55% 36% . 7% |
| 18  | u     | 104    |  52% 43% ..   |
| 19  | v     | 94     |  59% 39% .    |
| 20  | w     | 85     |  60% 28% 12%  |
| 21  | x     | 78     |  51% 46% ..   |
| 22  | y     | 63     |  71% 29%      |
| 23  | z     | 59     |  68% 29% ..   |
| 24  | B     | 57     |  54% 44% .    |
| 25  | C     | 55     |  56% 35% 9%   |
| 26  | D     | 46     |  61% 35% .    |
| 27  | E     | 65     |  57% 38% ..   |
| 28  | F     | 38     |  39% 61%      |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | G     | 241    |    |
| 30  | H     | 233    |    |
| 31  | I     | 206    |    |
| 32  | J     | 167    |    |
| 33  | K     | 131    |    |
| 34  | L     | 156    |    |
| 35  | M     | 130    |    |
| 36  | N     | 130    |    |
| 37  | O     | 103    |    |
| 38  | P     | 129    |    |
| 39  | Q     | 124    |    |
| 40  | R     | 118    |  |
| 41  | S     | 101    |  |
| 42  | T     | 89     |  |
| 43  | U     | 82     |  |
| 44  | V     | 84     |  |
| 45  | W     | 75     |  |
| 46  | X     | 92     |  |
| 47  | Y     | 87     |  |
| 48  | Z     | 71     |  |
| 49  | a     | 234    |  |
| 50  | 3     | 1539   |  |
| 51  | 1     | 2903   |  |
| 52  | 2     | 120    |  |
| 53  | 5     | 77     |  |

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| Mol | Chain | Length | Quality of chain                                                              |
|-----|-------|--------|-------------------------------------------------------------------------------|
| 54  | 4     | 27     | <div><div></div><div>41%</div><div>26%</div><div>7%</div><div>26%</div></div> |
| 55  | 8     | 371    | <div><div>24%</div><div>47%</div><div>46%</div><div>5%</div><div></div></div> |

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 147733 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     |
|     |       |          | 2082  | 1288 | 423 | 364 | 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     |
|     |       |          | 1410  | 899 | 249 | 256 | 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     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | j     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | k     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 938   | 587 | 180 | 165 | 6 |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | l     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | m     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | n     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 12  | o     | 116      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | p     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 14  | q     | 117      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | r     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | s     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | t     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 18  | u     | 102      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | v     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | w     | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 575   | 356 | 116 | 102 | 1 |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | x     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 22  | y     | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 23  | z     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 24  | B     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 25  | C     | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 263 | 75 | 71 |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | D     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 27  | E     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | F     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 29 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 29  | G     | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1756  | 1111 | 315 | 322 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 30  | H     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |       |

- Molecule 31 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 31  | I     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 32 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | J     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1156  | 719 | 218 | 213 | 6 |         |       |

- Molecule 33 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | K     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 824   | 520 | 149 | 149 | 6 |         |       |

- Molecule 34 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | L     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1181  | 735 | 227 | 215 | 4 |         |       |

- Molecule 35 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | M     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | N     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | O     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |       |

- Molecule 38 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | P     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 869   | 535 | 173 | 158 | 3 |         |       |

- Molecule 39 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | Q     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | R     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 883   | 546 | 178 | 156 | 3 |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | S     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | T     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | U     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | V     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |       |

- Molecule 45 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 45  | W     | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 535   | 339 | 100 | 95 | 1 |         |       |

- Molecule 46 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | X     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 637   | 408 | 120 | 107 | 2 |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | Y     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |       |

- Molecule 48 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 48  | Z     | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 544   | 335 | 117 | 91 | 1 |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | a     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1026  | 645 | 186 | 193 | 2 |         |       |

- Molecule 50 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 50  | 3     | 1539     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33012 | 14725 | 6052 | 10697 | 1538 |         |       |

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

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

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference     |
|-------|---------|----------|--------|----------|---------------|
| 1     | 747     | C        | U      | conflict | GB 1036415628 |

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

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

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference     |
|-------|---------|----------|--------|----------------|---------------|
| 2     | 120     | A        | -      | expression tag | GB 1370526515 |

- Molecule 53 is a RNA chain called tRNA<sup>fMet</sup>.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 53  | 5     | 73       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1556  | 694 | 281 | 509 | 72 |         |       |

- Molecule 54 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 54  | 4     | 20       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 437   | 197 | 91 | 130 | 19 |         |       |

- Molecule 55 is a protein called Peptide chain release factor 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 55  | 8     | 361      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2860  | 1758 | 503 | 589 | 10 |         |       |

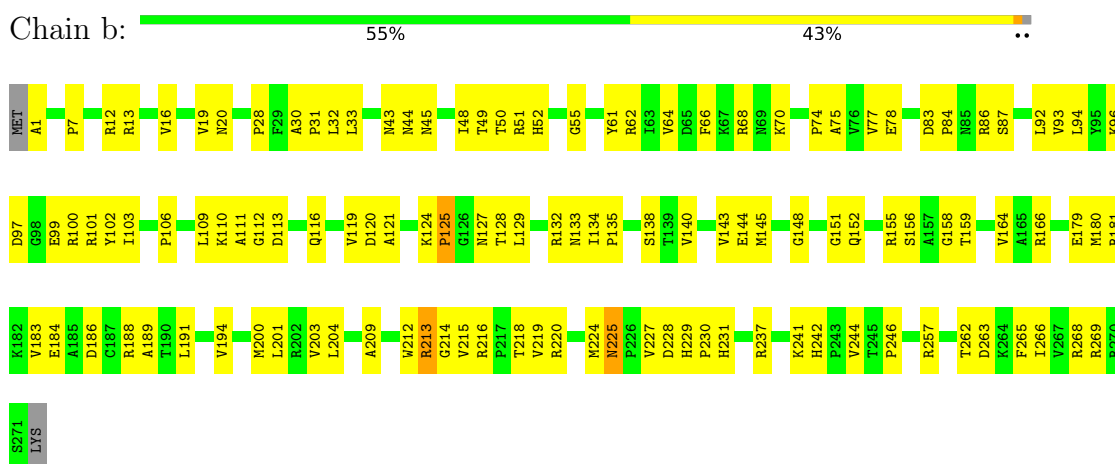
There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference      |
|-------|---------|----------|--------|-----------------------|----------------|
| 8     | -5      | MET      | -      | initiating methionine | UNP A0A2S5ZJX2 |
| 8     | -4      | HIS      | -      | expression tag        | UNP A0A2S5ZJX2 |
| 8     | -3      | HIS      | -      | expression tag        | UNP A0A2S5ZJX2 |
| 8     | -2      | HIS      | -      | expression tag        | UNP A0A2S5ZJX2 |
| 8     | -1      | HIS      | -      | expression tag        | UNP A0A2S5ZJX2 |
| 8     | 0       | HIS      | -      | expression tag        | UNP A0A2S5ZJX2 |
| 8     | 1       | HIS      | -      | expression tag        | UNP A0A2S5ZJX2 |

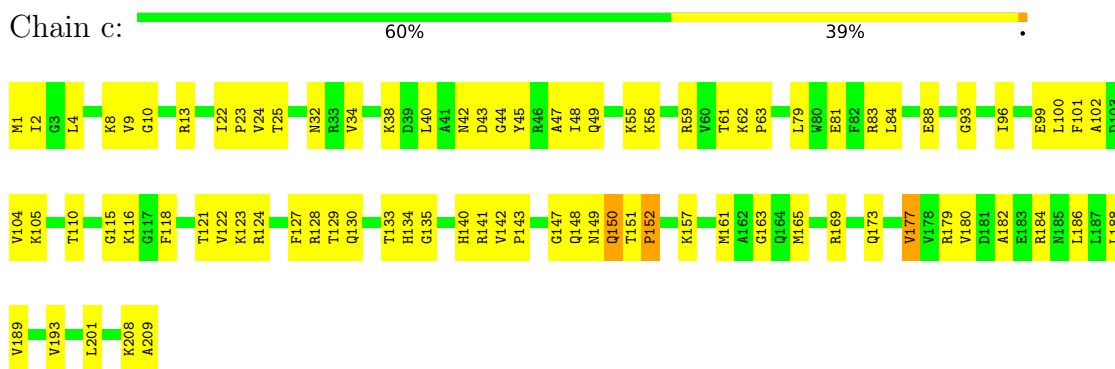
### 3 Residue-property plots

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.

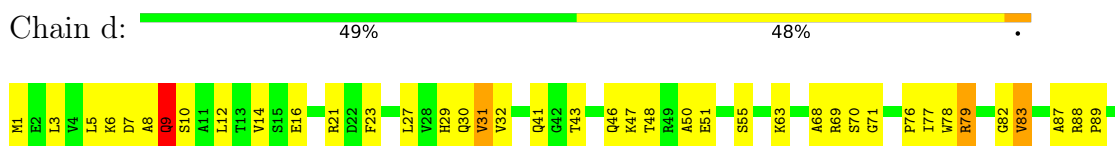
#### • Molecule 1: 50S ribosomal protein L2

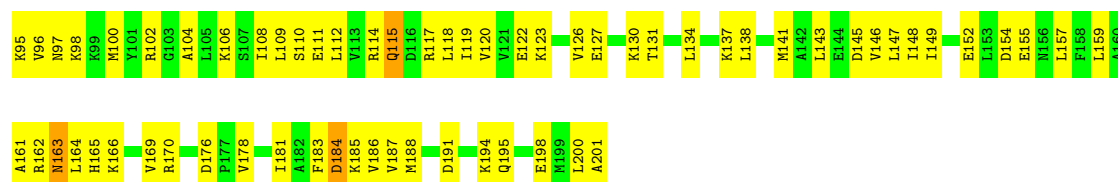


#### • Molecule 2: 50S ribosomal protein L3



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





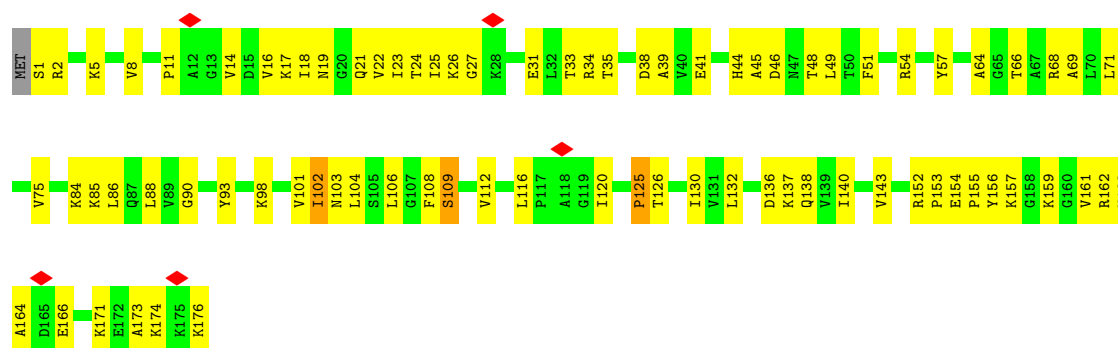
• Molecule 4: 50S ribosomal protein L5

Chain e: 42% 55%



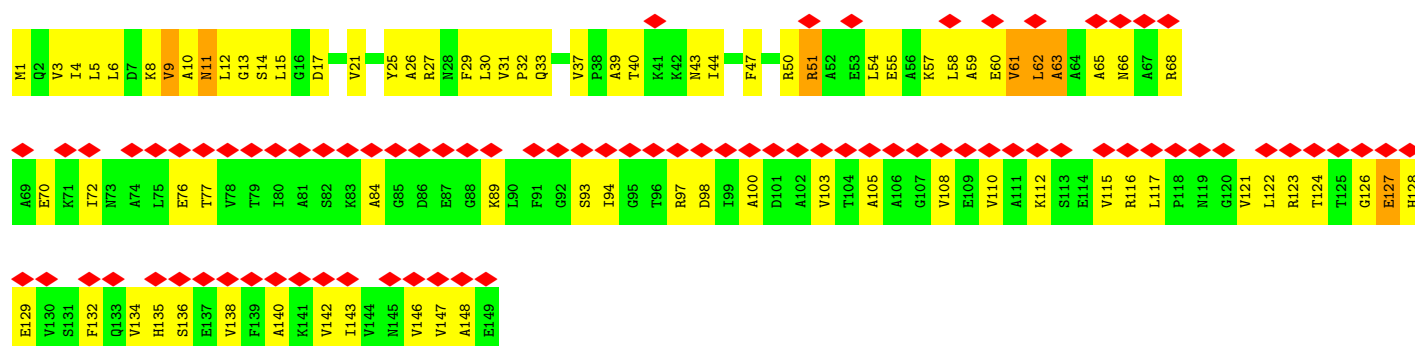
• Molecule 5: 50S ribosomal protein L6

Chain f: 54% 44%



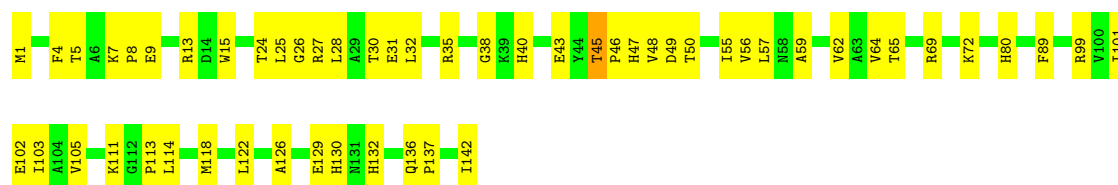
• Molecule 6: 50S ribosomal protein L9

Chain g: 56% 46% 50% 5%



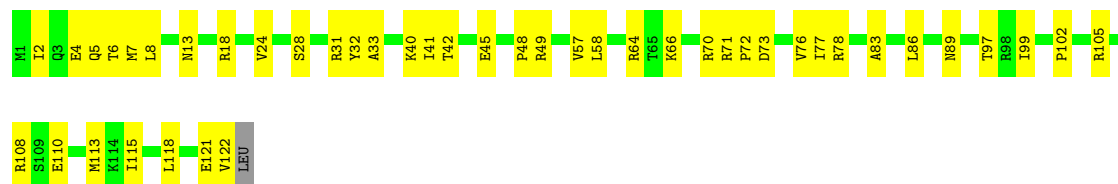
• Molecule 7: 50S ribosomal protein L13

Chain j: 



- Molecule 8: 50S ribosomal protein L14

Chain k: 



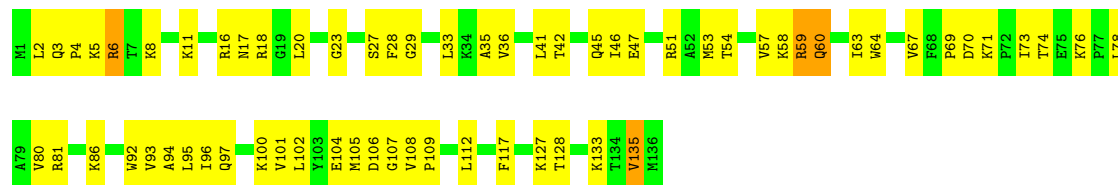
- Molecule 9: 50S ribosomal protein L15

Chain l: 



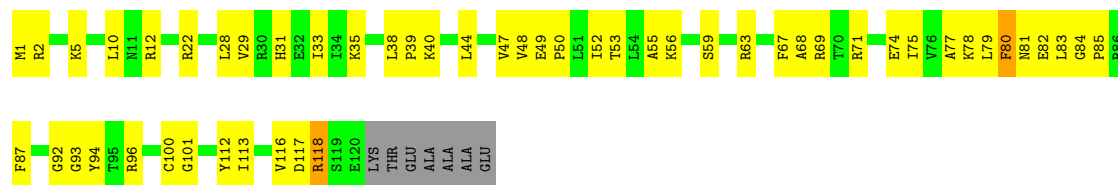
- Molecule 10: 50S ribosomal protein L16

Chain m: 



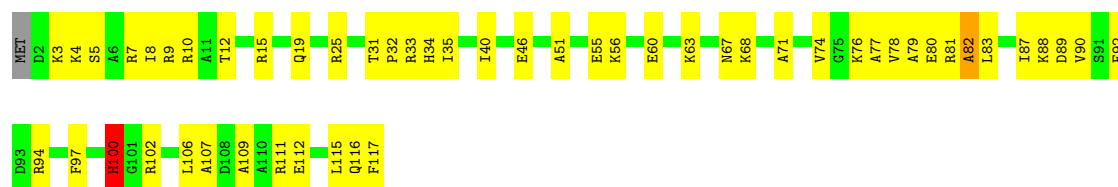
- Molecule 11: 50S ribosomal protein L17

Chain n: 



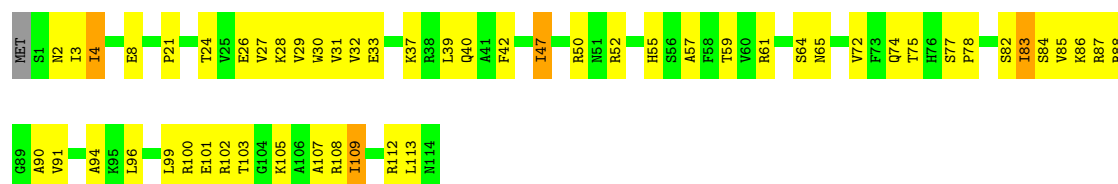
- Molecule 12: 50S ribosomal protein L18

Chain o:  55% 43% ...



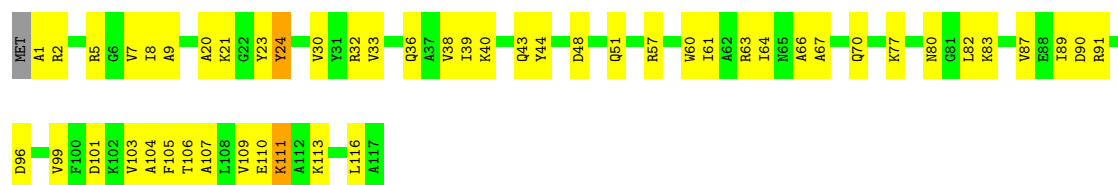
- Molecule 13: 50S ribosomal protein L19

Chain p:  52% 43% ..



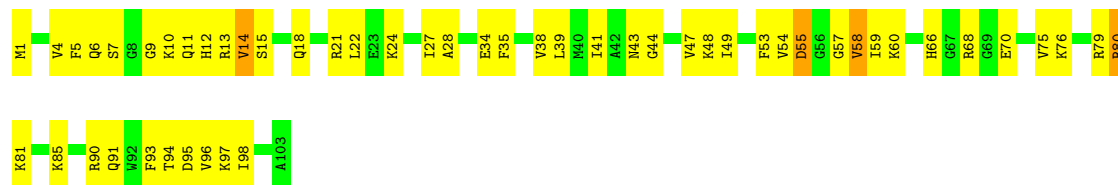
- Molecule 14: 50S ribosomal protein L20

Chain q:  57% 41% ..



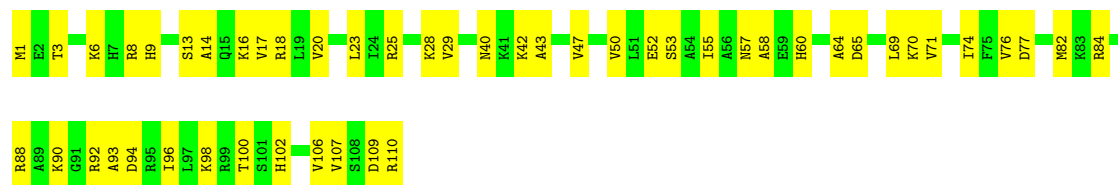
- Molecule 15: 50S ribosomal protein L21

Chain r:  50% 47% .



- Molecule 16: 50S ribosomal protein L22

Chain s:  55% 45%



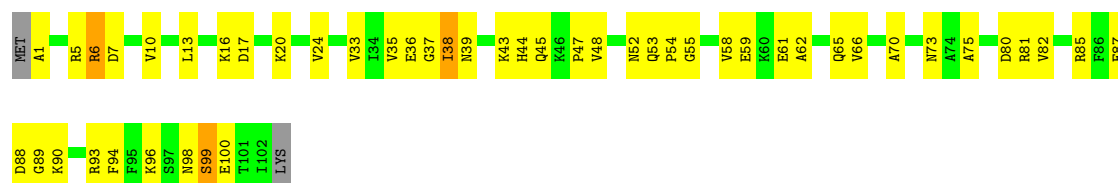
- Molecule 17: 50S ribosomal protein L23

Chain t:  55% 36% 7%



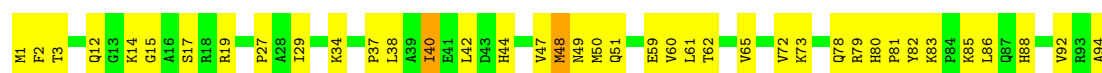
• Molecule 18: 50S ribosomal protein L24

Chain u:  52% 43% 2%



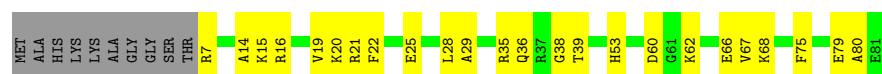
• Molecule 19: 50S ribosomal protein L25

Chain v:  59% 39% 2%



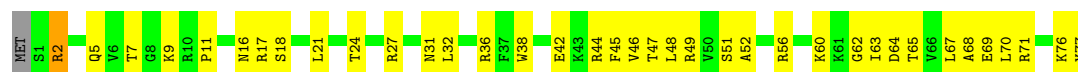
• Molecule 20: 50S ribosomal protein L27

Chain w:  60% 28% 12%



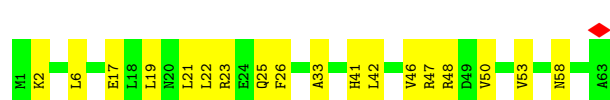
• Molecule 21: 50S ribosomal protein L28

Chain x:  51% 46% 3%



• Molecule 22: 50S ribosomal protein L29

Chain y:  71% 29% 0%

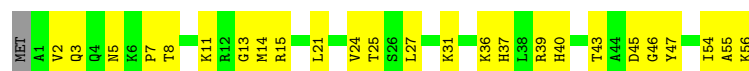


• Molecule 23: 50S ribosomal protein L30

Chain z:  68% 29% 3%



- Molecule 24: 50S ribosomal protein L32



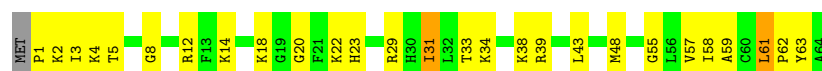
- Molecule 25: 50S ribosomal protein L33



- Molecule 26: 50S ribosomal protein L34



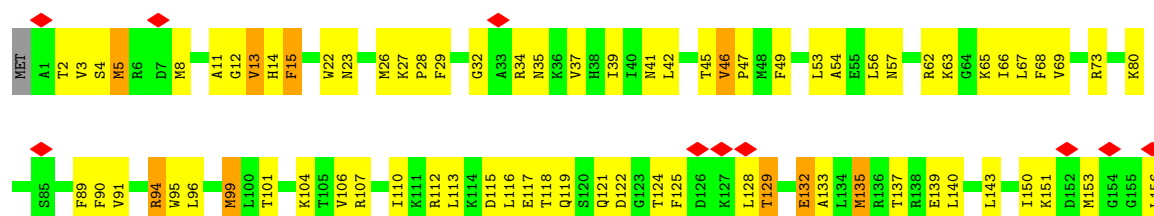
- Molecule 27: 50S ribosomal protein L35

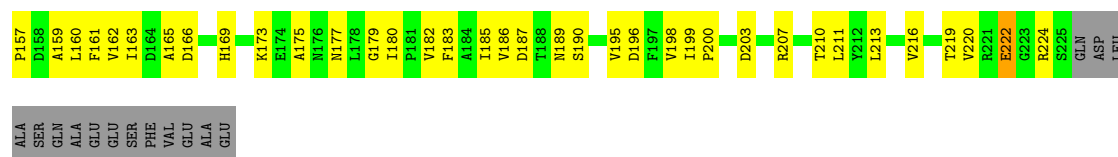


- Molecule 28: 50S ribosomal protein L36

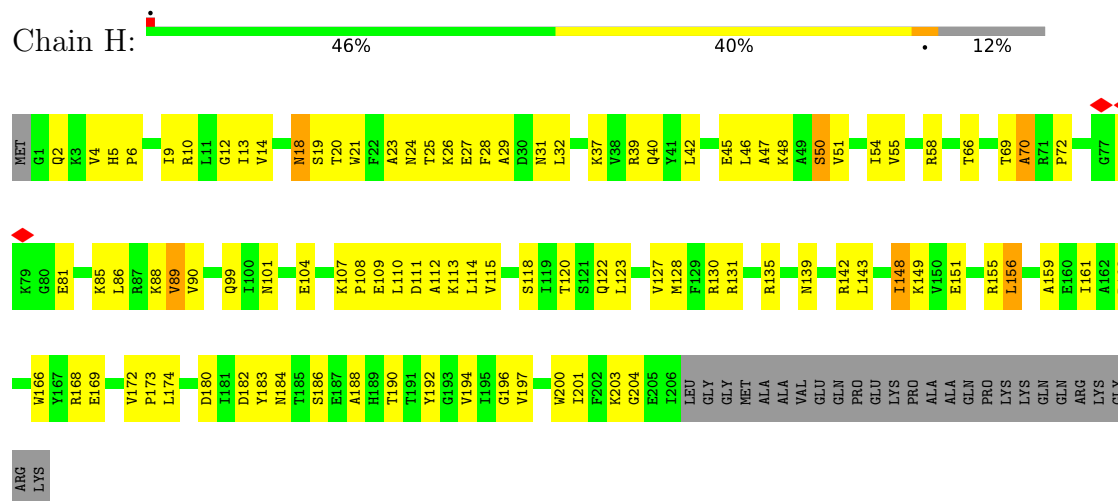


- Molecule 29: 30S ribosomal protein S2

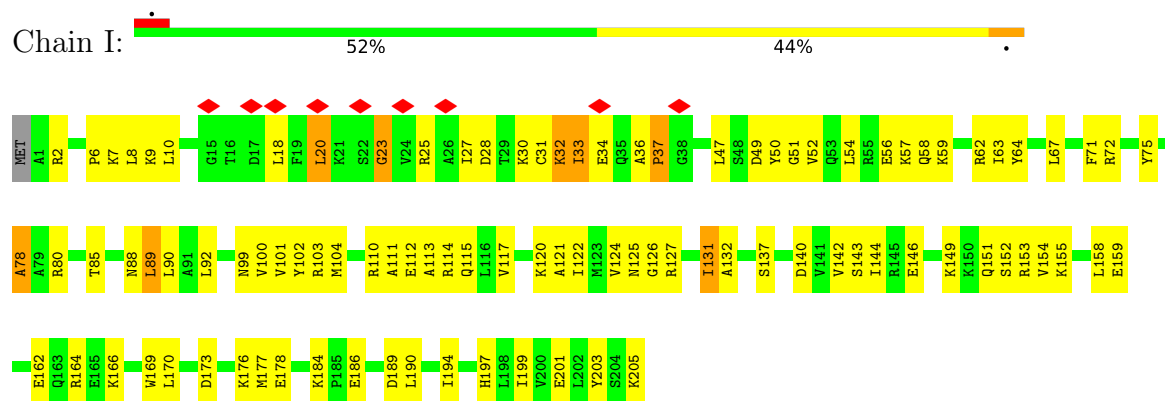




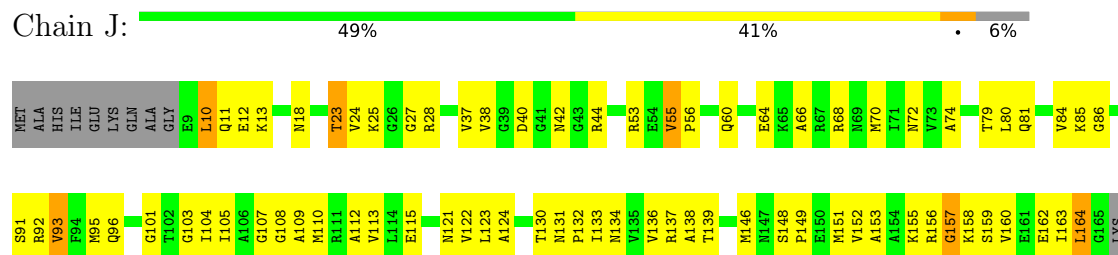
• Molecule 30: 30S ribosomal protein S3



• Molecule 31: 30S ribosomal protein S4

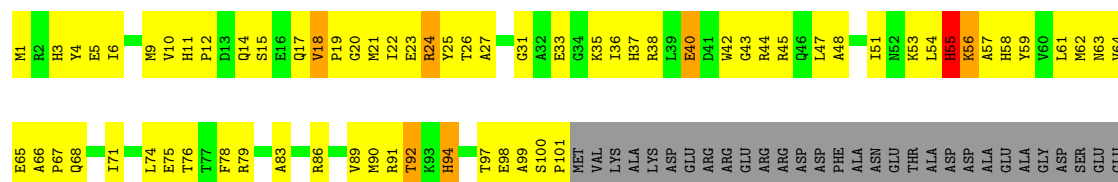


• Molecule 32: 30S ribosomal protein S5

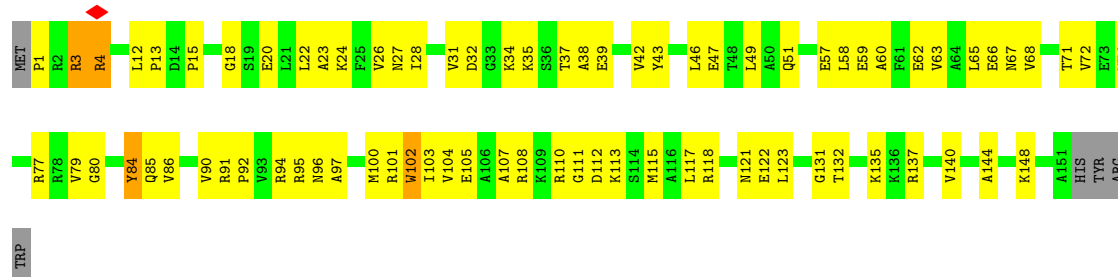


• Molecule 33: 30S ribosomal protein S6

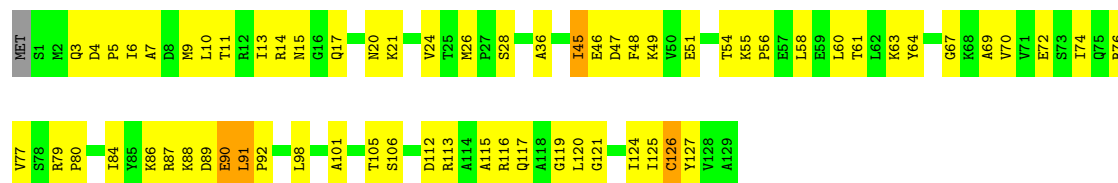




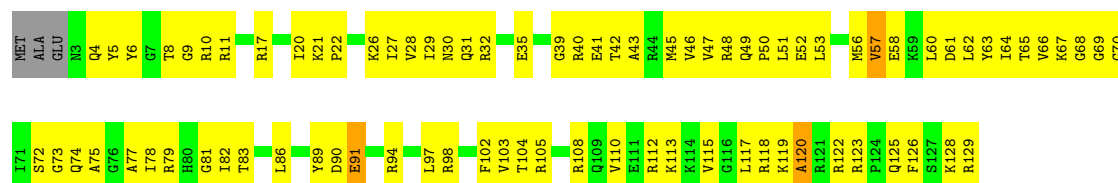
• Molecule 34: 30S ribosomal protein S7



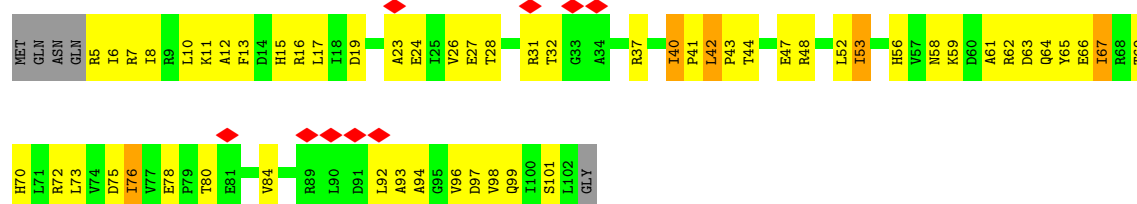
• Molecule 35: 30S ribosomal protein S8



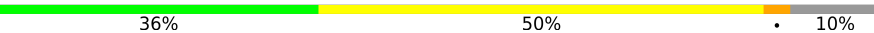
• Molecule 36: 30S ribosomal protein S9

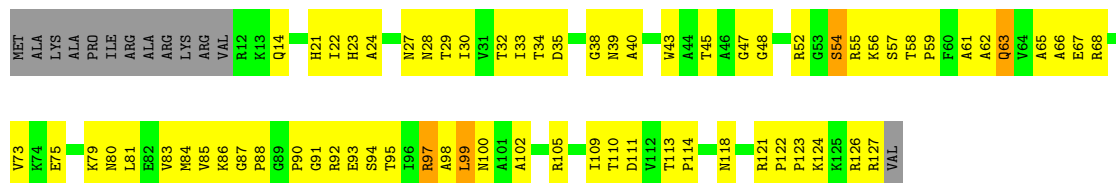


• Molecule 37: 30S ribosomal protein S10

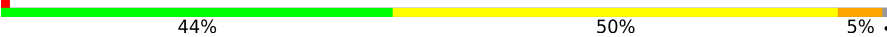


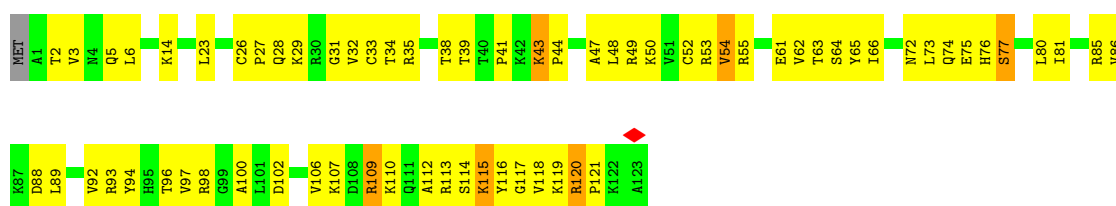
- Molecule 38: 30S ribosomal protein S11

Chain P:  36% 50% 10%



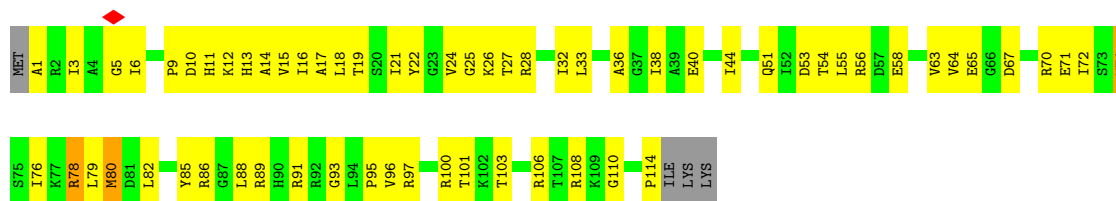
- Molecule 39: 30S ribosomal protein S12

Chain Q:  44% 50% 5%



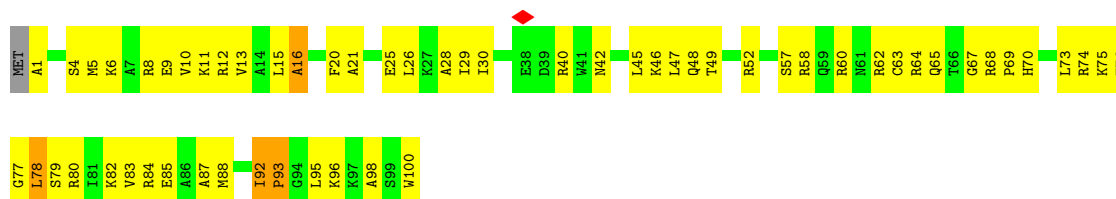
- Molecule 40: 30S ribosomal protein S13

Chain R:  43% 51% 4% 2%



- Molecule 41: 30S ribosomal protein S14

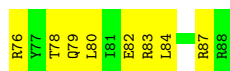
Chain S:  42% 53% 3% 2%



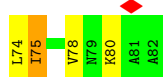
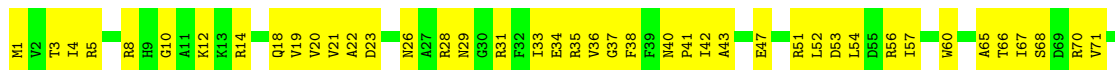
- Molecule 42: 30S ribosomal protein S15

Chain T:  46% 48% 4% 2%

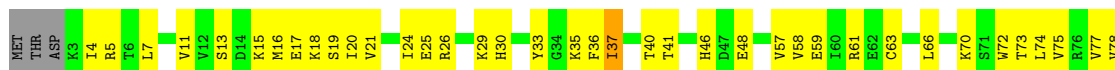




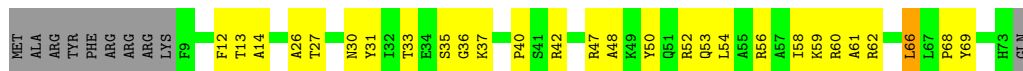
- Molecule 43: 30S ribosomal protein S16



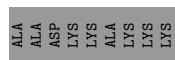
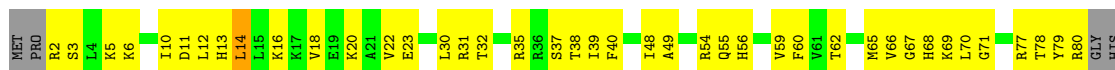
- Molecule 44: 30S ribosomal protein S17



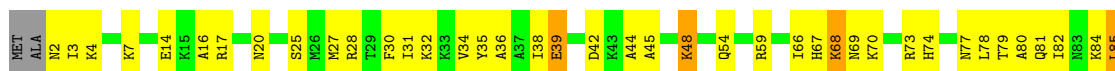
- Molecule 45: 30S ribosomal protein S18



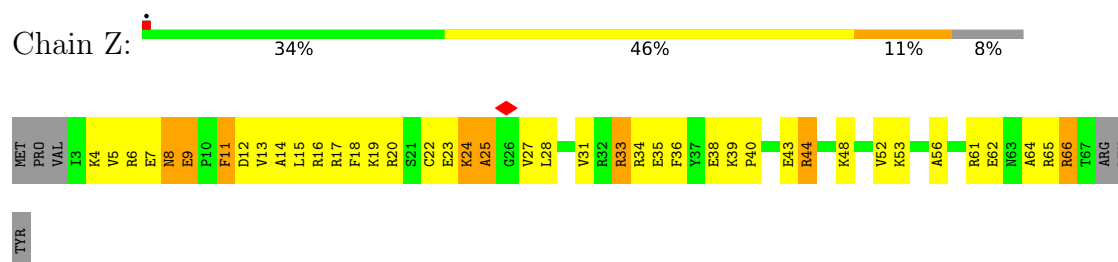
- Molecule 46: 30S ribosomal protein S19



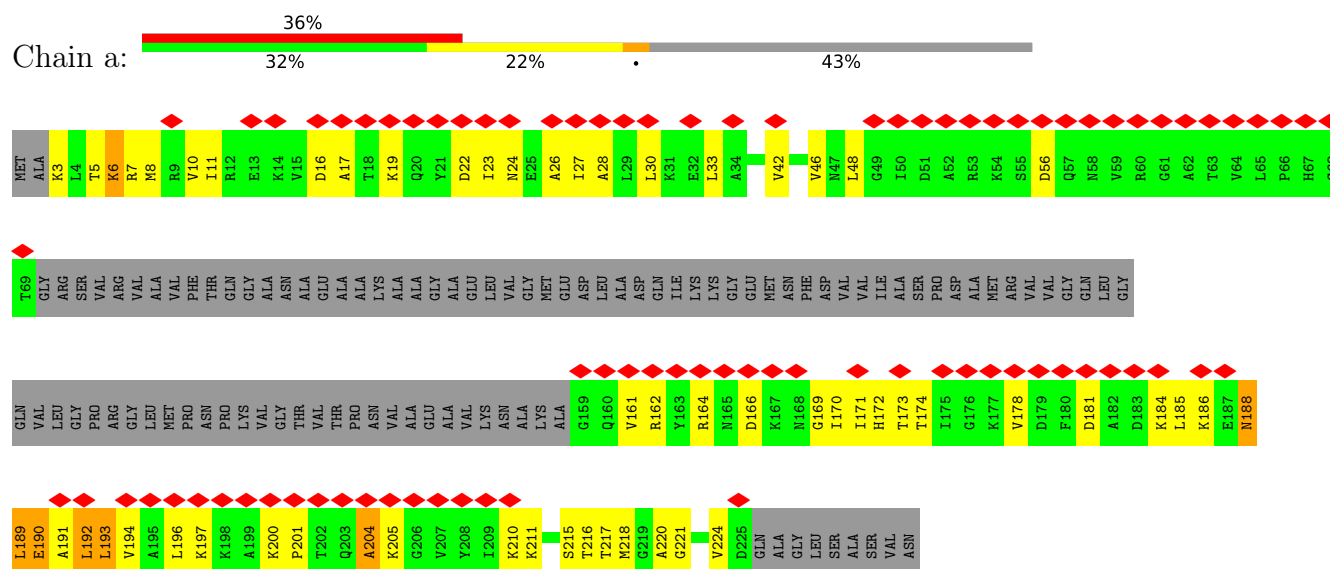
- Molecule 47: 30S ribosomal protein S20



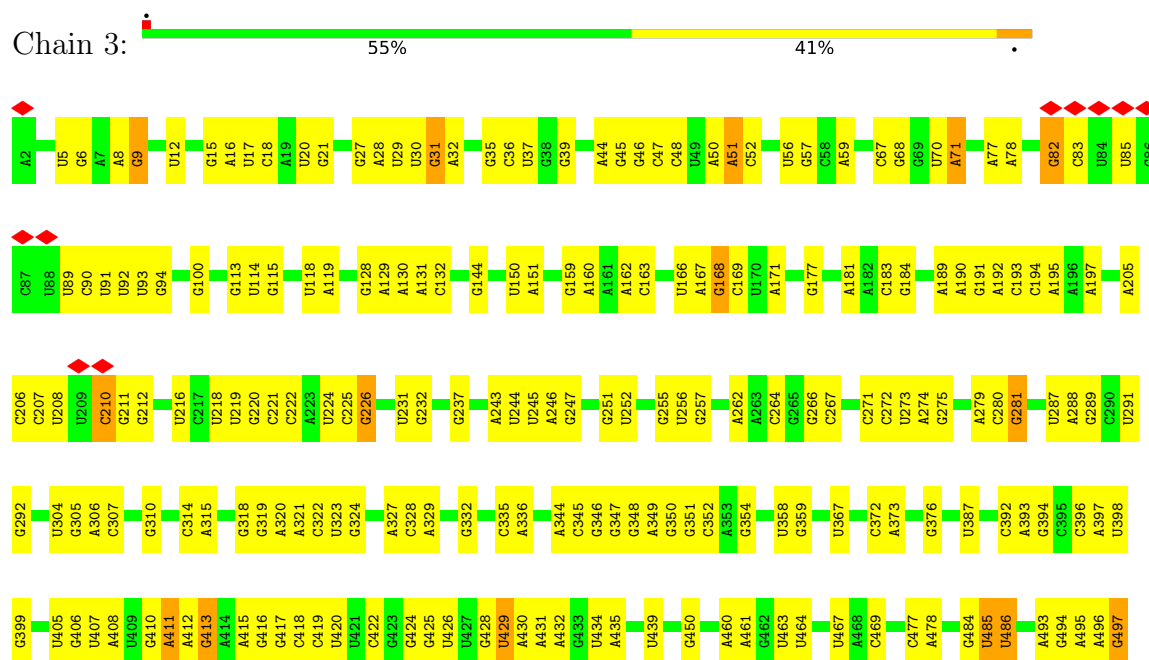
- Molecule 48: 30S ribosomal protein S21

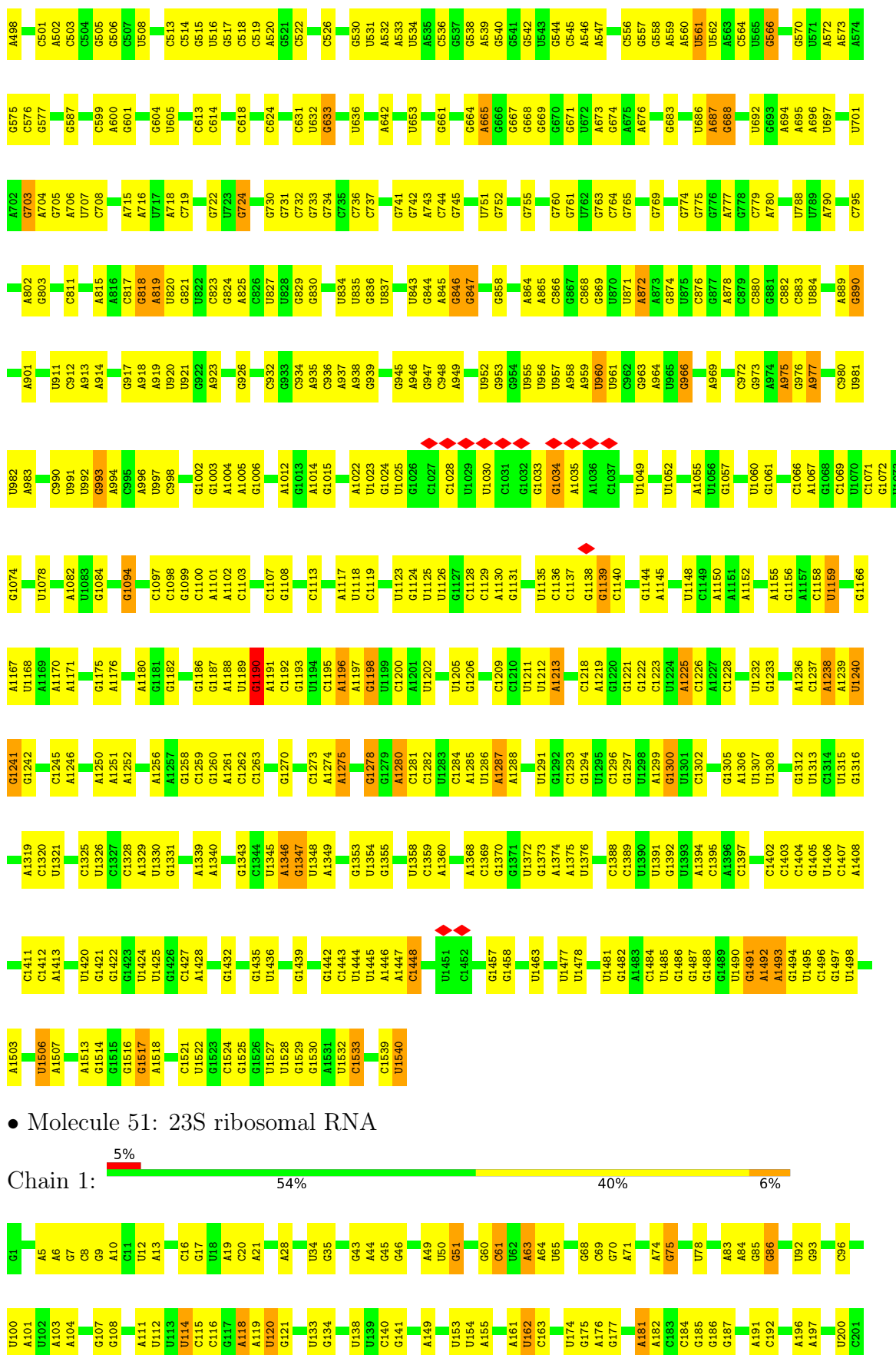


- Molecule 49: 50S ribosomal protein L1



- Molecule 50: 16S ribosomal RNA

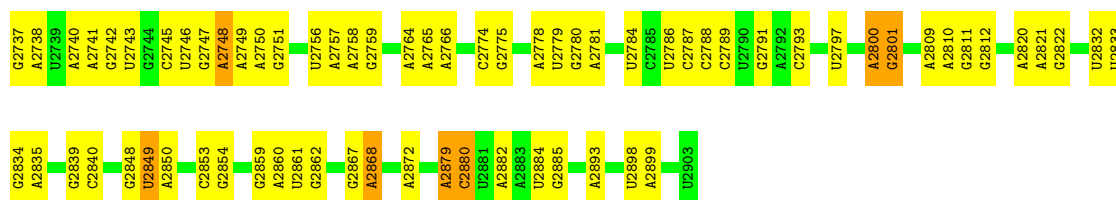




• Molecule 51: 23S ribosomal RNA

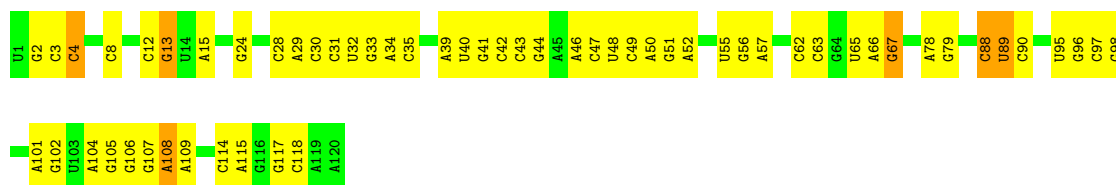
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G1441 | U1442 | U1443 | G1444 | G1447 | G1448 | G1449 | G1450 | C1451 | G1452 | A1453 | G1454 | G1455 | U1458 | G1459 | C1460 | C1461 | G1465 | U1466 | U1467 | U1468 | A1469 | A1470 | G1471 | G1472 | G1473 | G1475 | U1476 | A1477 | G1478 | G1479 | U1480 | U1481 | G1482 | G1483 | G1484 | U1485 | U1486 | U1487 | C1488 | C1489 | A1490 | G1491 | G1492 | C1493 | A1494 | A1495 | A1496 | U1497 | C1498 | C1499 | G1500 | A1501 | A1502 | A1503 | A1504 |
| U1340 | G1341 | G1341 | U1344 | C1345 | G1337 | G1338 | G1339 | C1357 | G1358 | A1365 | A1366 | A1367 | G1368 | G1369 | U1265 | G1370 | U1378 | U1379 | A1383 | C1386 | A1387 | U1394 | U1397 | C1398 | U1406 | U1409 | G1410 | U1415 | G1416 | C1417 | G1418 | A1419 | A1420 | G1421 | G1422 | G1423 | G1424 | G1425 | G1426 | A1427 | C1428 | G1429 | G1430 | A1431 | G1432 | A1433 | C1437 | U1438 | A1439 | U1440 |       |       |       |       |       |
| U1231 | G1232 | G1236 | G1239 | U1240 | G1243 | G1248 | G1252 | A1253 | U1254 | U1255 | G1256 | C1257 | U1258 | G1259 | A1260 | A1268 | A1269 | C1270 | G1271 | A1272 | C1278 | G1279 | U1282 | G1283 | A1284 | A1285 | A1286 | A1287 | G1288 | C1289 | C1297 | G1298 | G1299 | G1300 | A1301 | G1311 | U1316 | G1317 | U1318 | G1319 | C1320 | C1321 | A1321 | U1326 | A1327 | A1328 | U1329 | C1330 |       |       |       |       |       |       |       |
| U1131 | U1132 | C1135 | G1136 | G1137 | G1138 | G1139 | U1141 | U1141 | A1142 | A1143 | A1147 | U1148 | G1149 | C1150 | A1151 | G1152 | U1153 | G1154 | G1157 | C1161 | G1162 | G1168 | G1171 | C1172 | U1173 | U1174 | A1175 | U1176 | G1177 | C1178 | G1179 | U1180 | U1181 | G1185 | G1186 | G1187 | G1190 | G1191 | C1196 | G1197 | G1210 | C1211 | G1212 | A1213 | A1214 | G1215 | C1229 | A1230 |       |       |       |       |       |       |       |
| C1053 | A1057 | U1058 | G1059 | U1060 | U1061 | G1062 | G1063 | C1064 | U1065 | U1066 | A1067 | G1068 | A1069 | A1070 | G1071 | C1072 | A1073 | G1074 | C1075 | U1078 | C1079 | U1080 | U1081 | U1082 | U1083 | A1084 | A1085 | A1086 | G1087 | A1088 | A1089 | G1093 | U1094 | A1095 | A1096 | U1097 | A1098 | U1099 | C1100 | U1101 | C1102 | C1103 | C1104 | U1105 | G1110 | A1111 | G1112 | U1113 | U1119 |       |       |       |       |       |       |
| C961  | G962  | U963  | U967  | C968  | G969  | U970  | G971  | A972  | A973  | G974  | A975  | A983  | C987  | C988  | C989  | A990  | C991  | C992  | G993  | C994  | C995  | A996  | G997  | C1005 | A1009 | A1010 | G1011 | U1012 | C1013 | A1020 | A1021 | G1022 | U1023 | G1024 | G1025 | G1026 | A1027 | A1028 | A1029 | U1033 | A1040 | C1043 | C1044 | C1045 | A1046 | G1047 | A1048 | A1050 |       |       |       |       |       |       |       |
| U860  | A861  | G862  | A863  | G869  | G875  | C876  | A877  | A878  | U884  | C885  | A886  | U887  | C888  | C889  | C890  | G891  | A892  | C893  | A896  | A899  | G901  | C902  | A905  | U906  | A910  | C912  | U913  | A917  | C922  | A928  | U931  | U932  | G940  | A941  | G942  | A943  | C946  | A947  | C948  | G949  | U955  | G956  |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G776  | A781  | A782  | A783  | G784  | G785  | G791  | A792  | A793  | G796  | G797  | G798  | A800  | U803  | A804  | G805  | C806  | U807  | G808  | G809  | U810  | U811  | C812  | U813  | C814  | C817  | G818  | A819  | U826  | U827  | U828  | G830  | G831  | U832  | A833  | U839  | C840  | A845  | U846  | U847  | C851  | U852  | C853  | C854  | G855  | G856  | G857  | G858  | G859  |       |       |       |       |       |       |       |
| A668  | G669  | A670  | C671  | C672  | C673  | G674  | C679  | C680  | A686  | U686  | C687  | U688  | G695  | G700  | G701  | U702  | U703  | G704  | C717  | A718  | C719  | U720  | A721  | G726  | A727  | G728  | G729  | A730  | G738  | A739  | C740  | U741  | A742  | A743  | U744  | G745  | U746  | C747  | G748  | A751  | A752  | G763  | A764  | U767  | G768  | G774  | G775  |       |       |       |       |       |       |       |       |
| U580  | C581  | A582  | G583  | C584  | G585  | A586  | C587  | U588  | U591  | A592  | A593  | U594  | C595  | U596  | G597  | U598  | A599  | A603  | A609  | C610  | U615  | A616  | G617  | A626  | A627  | A631  | A632  | A633  | C634  | C635  | G636  | A637  | G638  | U639  | C640  | U646  | G647  | G651  | A654  | A655  | G656  | U657  | U658  | G659  | G662  | G663  | A666  | U667  |       |       |       |       |       |       |       |
| G491  | A492  | G493  | G494  | G495  | G498  | A503  | A504  | A505  | G506  | A507  | A508  | U511  | G512  | A513  | G518  | A528  | A529  | G530  | C531  | A532  | G533  | G537  | U545  | U546  | A547  | G548  | G549  | C550  | U554  | G555  | U558  | G559  | U562  | A563  | C564  | U565  | A654  | A655  | G656  | U657  | U658  | G659  | G662  | G663  | A666  | U667  |       |       |       |       |       |       |       |       |       |
| A310  | A311  | G312  | A320  | U321  | A322  | C323  | A324  | G325  | A326  | G327  | U328  | G329  | A330  | A340  | A341  | A345  | A346  | A347  | A348  | G351  | A352  | C357  | U358  | G359  | U360  | A361  | A362  | G363  | C366  | G367  | A368  | U369  | G370  | A371  | G372  | U373  | G380  | G386  | U387  | G388  | G389  | U390  | A391  | U392  | A483  | C394  | U395  | G396  | G400  | A401  |       |       |       |       |       |
| A402  | U403  | A404  | U405  | G406  | G407  | G411  | A412  | C413  | A414  | A415  | U419  | C420  | A421  | G424  | C433  | U434  | C435  | C436  | U437  | G438  | A439  | C440  | U441  | G442  | C445  | C446  | U448  | A449  | U451  | C456  | A457  | A466  | G467  | G468  | G469  | A470  | A477  | A478  | A479  | A480  | U481  | A482  | A483  | C484  | C487  | G488  | G489  | C490  |       |       |       |       |       |       |       |
| U202  | A203  | A204  | G205  | C210  | C211  | G214  | G215  | A216  | A221  | A222  | C225  | A226  | A227  | C228  | C229  | A231  | G242  | G247  | G248  | G254  | A255  | A256  | G259  | G260  | A265  | G266  | C275  | U276  | G277  | A278  | A279  | U280  | C281  | U288  | G289  | U290  | U296  | G297  | G298  | A299  | A300  | U306  | G307  | G308  | A309  |       |       |       |       |       |       |       |       |       |       |





• Molecule 52: 5S ribosomal RNA

Chain 2: 52% 43% 5%



• Molecule 53: tRNA<sup>fMet</sup>

Chain 5: 12% 61% 32% 5%



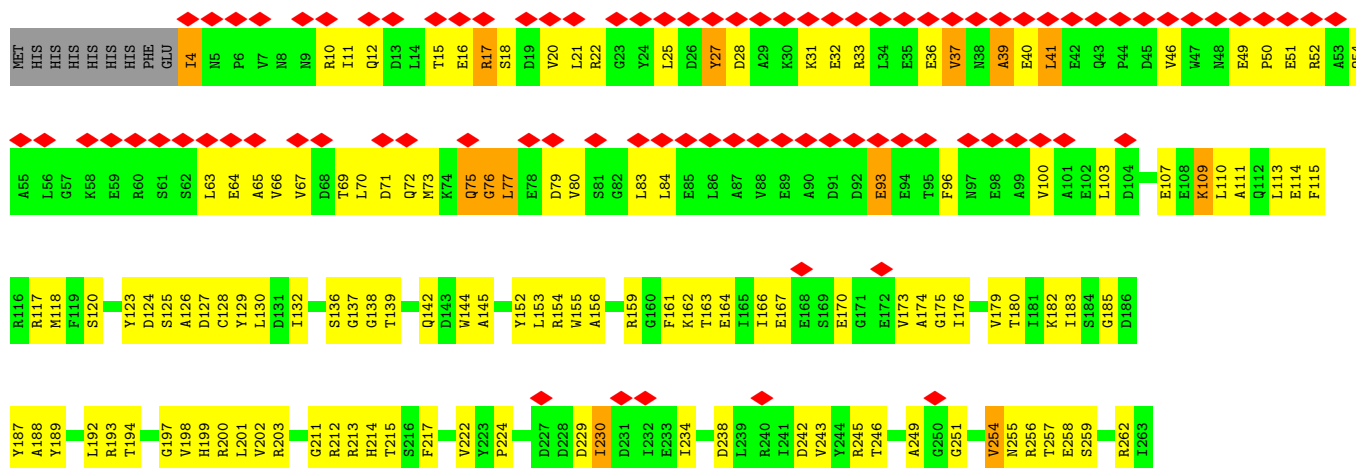
• Molecule 54: mRNA

Chain 4: 41% 26% 7% 26%



• Molecule 55: Peptide chain release factor 2

Chain 8: 24% 47% 46% 5%





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 28549                                   | 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 ( $e^-/\text{\AA}^2$ ) | 29.4                                    | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 7.540                                   | Depositor |
| Minimum map value                    | -2.221                                  | Depositor |
| Average map value                    | 0.005                                   | Depositor |
| Map value standard deviation         | 0.481                                   | Depositor |
| Recommended contour level            | 0.9                                     | Depositor |
| Map size (Å)                         | 416.208, 416.208, 416.208               | wwPDB     |
| Map dimensions                       | 312, 312, 312                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.334, 1.334, 1.334                     | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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     | 0.29         | 0/2121  | 0.84        | 5/2852 (0.2%) |
| 2   | c     | 0.30         | 0/1586  | 0.85        | 3/2134 (0.1%) |
| 3   | d     | 0.29         | 0/1571  | 0.86        | 7/2113 (0.3%) |
| 4   | e     | 0.31         | 0/1434  | 0.95        | 8/1926 (0.4%) |
| 5   | f     | 0.31         | 0/1343  | 0.86        | 1/1816 (0.1%) |
| 6   | g     | 0.33         | 0/1122  | 1.00        | 6/1515 (0.4%) |
| 7   | j     | 0.30         | 0/1152  | 0.89        | 3/1551 (0.2%) |
| 8   | k     | 0.27         | 0/947   | 0.89        | 1/1268 (0.1%) |
| 9   | l     | 0.30         | 0/1054  | 0.92        | 5/1403 (0.4%) |
| 10  | m     | 0.31         | 0/1093  | 0.86        | 3/1460 (0.2%) |
| 11  | n     | 0.29         | 0/973   | 0.88        | 3/1301 (0.2%) |
| 12  | o     | 0.30         | 0/902   | 0.85        | 1/1209 (0.1%) |
| 13  | p     | 0.30         | 0/929   | 0.86        | 1/1242 (0.1%) |
| 14  | q     | 0.29         | 0/960   | 0.90        | 3/1278 (0.2%) |
| 15  | r     | 0.30         | 0/829   | 0.88        | 4/1107 (0.4%) |
| 16  | s     | 0.31         | 0/864   | 0.86        | 2/1156 (0.2%) |
| 17  | t     | 0.28         | 0/744   | 0.80        | 0/994         |
| 18  | u     | 0.29         | 0/787   | 0.83        | 1/1051 (0.1%) |
| 19  | v     | 0.31         | 0/766   | 0.84        | 3/1025 (0.3%) |
| 20  | w     | 0.29         | 0/582   | 0.83        | 1/769 (0.1%)  |
| 21  | x     | 0.30         | 0/635   | 0.86        | 1/848 (0.1%)  |
| 22  | y     | 0.28         | 0/510   | 0.92        | 0/677         |
| 23  | z     | 0.29         | 0/453   | 0.82        | 0/605         |
| 24  | B     | 0.28         | 0/450   | 0.80        | 0/599         |
| 25  | C     | 0.31         | 0/416   | 0.71        | 0/554         |
| 26  | D     | 0.30         | 0/380   | 0.93        | 2/498 (0.4%)  |
| 27  | E     | 0.29         | 0/513   | 0.86        | 2/676 (0.3%)  |
| 28  | F     | 0.33         | 0/303   | 0.92        | 2/397 (0.5%)  |
| 29  | G     | 0.32         | 0/1787  | 0.96        | 8/2408 (0.3%) |
| 30  | H     | 0.32         | 0/1651  | 0.86        | 5/2225 (0.2%) |
| 31  | I     | 0.29         | 0/1665  | 0.96        | 7/2227 (0.3%) |
| 32  | J     | 0.33         | 0/1169  | 0.97        | 5/1573 (0.3%) |
| 33  | K     | 0.31         | 0/843   | 0.97        | 5/1140 (0.4%) |
| 34  | L     | 0.29         | 0/1195  | 0.97        | 5/1602 (0.3%) |

| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 35  | M     | 0.30         | 0/989    | 0.94        | 6/1326 (0.5%)     |
| 36  | N     | 0.31         | 0/1034   | 0.96        | 3/1375 (0.2%)     |
| 37  | O     | 0.32         | 0/796    | 0.92        | 3/1077 (0.3%)     |
| 38  | P     | 0.33         | 0/885    | 1.07        | 10/1195 (0.8%)    |
| 39  | Q     | 0.31         | 0/969    | 1.06        | 6/1300 (0.5%)     |
| 40  | R     | 0.30         | 0/892    | 0.97        | 5/1193 (0.4%)     |
| 41  | S     | 0.29         | 0/817    | 1.00        | 3/1088 (0.3%)     |
| 42  | T     | 0.30         | 0/722    | 1.01        | 4/964 (0.4%)      |
| 43  | U     | 0.32         | 0/659    | 0.87        | 1/884 (0.1%)      |
| 44  | V     | 0.30         | 0/657    | 0.82        | 1/881 (0.1%)      |
| 45  | W     | 0.31         | 0/544    | 0.95        | 3/731 (0.4%)      |
| 46  | X     | 0.33         | 0/652    | 0.86        | 0/877             |
| 47  | Y     | 0.29         | 0/671    | 0.95        | 3/888 (0.3%)      |
| 48  | Z     | 0.34         | 0/550    | 1.10        | 6/728 (0.8%)      |
| 49  | a     | 0.33         | 0/1033   | 1.00        | 11/1387 (0.8%)    |
| 50  | 3     | 0.41         | 0/36963  | 0.46        | 1/57662 (0.0%)    |
| 51  | 1     | 0.40         | 0/69796  | 0.47        | 1/108888 (0.0%)   |
| 52  | 2     | 0.42         | 0/2872   | 0.46        | 0/4479            |
| 53  | 5     | 0.42         | 0/1738   | 0.46        | 0/2709            |
| 54  | 4     | 0.39         | 0/493    | 0.49        | 0/769             |
| 55  | 8     | 0.30         | 0/2900   | 1.00        | 25/3908 (0.6%)    |
| All | All   | 0.38         | 0/160361 | 0.62        | 195/239508 (0.1%) |

There are no bond length outliers.

All (195) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 38  | P     | 99  | LEU  | N-CA-C | -9.30 | 102.07      | 113.41   |
| 39  | Q     | 109 | ARG  | N-CA-C | -8.90 | 95.25       | 109.59   |
| 42  | T     | 43  | ALA  | N-CA-C | -8.80 | 101.61      | 111.82   |
| 10  | m     | 60  | GLN  | N-CA-C | 8.69  | 121.53      | 110.24   |
| 48  | Z     | 17  | ARG  | N-CA-C | -8.67 | 100.10      | 113.02   |
| 9   | l     | 96  | LYS  | N-CA-C | -8.64 | 101.80      | 111.82   |
| 6   | g     | 61  | VAL  | N-CA-C | -8.16 | 101.15      | 112.50   |
| 37  | O     | 53  | ILE  | N-CA-C | 8.10  | 118.78      | 111.81   |
| 3   | d     | 165 | HIS  | N-CA-C | 8.08  | 119.72      | 111.07   |
| 39  | Q     | 114 | SER  | N-CA-C | -7.87 | 102.64      | 111.14   |
| 29  | G     | 13  | VAL  | N-CA-C | -7.65 | 105.10      | 111.91   |
| 39  | Q     | 120 | ARG  | N-CA-C | 7.55  | 120.44      | 109.71   |
| 6   | g     | 27  | ARG  | N-CA-C | 7.49  | 120.32      | 111.71   |
| 4   | e     | 169 | LEU  | N-CA-C | -7.47 | 102.82      | 112.23   |
| 15  | r     | 44  | GLY  | N-CA-C | -7.32 | 103.94      | 112.73   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | 8     | 229  | ASP  | N-CA-C      | 7.32  | 118.17      | 108.07   |
| 29  | G     | 222  | GLU  | N-CA-C      | -7.21 | 104.29      | 113.23   |
| 45  | W     | 14   | ALA  | N-CA-C      | -7.10 | 102.95      | 111.69   |
| 35  | M     | 6    | ILE  | N-CA-C      | 6.93  | 117.44      | 110.23   |
| 42  | T     | 39   | GLN  | N-CA-C      | -6.90 | 103.84      | 111.36   |
| 55  | 8     | 254  | VAL  | N-CA-C      | 6.86  | 119.02      | 109.55   |
| 41  | S     | 49   | THR  | N-CA-C      | -6.82 | 103.91      | 111.82   |
| 13  | p     | 33   | GLU  | N-CA-C      | -6.78 | 102.11      | 110.65   |
| 48  | Z     | 33   | ARG  | N-CA-C      | 6.71  | 116.84      | 108.19   |
| 33  | K     | 27   | ALA  | N-CA-C      | -6.68 | 104.08      | 111.36   |
| 49  | a     | 190  | GLU  | N-CA-C      | -6.67 | 103.48      | 111.69   |
| 49  | a     | 188  | ASN  | N-CA-C      | -6.67 | 103.83      | 112.23   |
| 6   | g     | 105  | ALA  | N-CA-C      | -6.66 | 104.63      | 112.89   |
| 34  | L     | 3    | ARG  | N-CA-C      | 6.65  | 121.13      | 111.02   |
| 34  | L     | 71   | THR  | N-CA-C      | -6.62 | 107.07      | 114.62   |
| 55  | 8     | 275  | GLN  | N-CA-C      | -6.61 | 104.53      | 112.59   |
| 39  | Q     | 115  | LYS  | N-CA-C      | -6.60 | 100.52      | 110.28   |
| 38  | P     | 67   | GLU  | N-CA-C      | -6.56 | 104.76      | 112.89   |
| 16  | s     | 60   | HIS  | N-CA-C      | 6.42  | 119.58      | 111.69   |
| 36  | N     | 126  | PHE  | N-CA-C      | 6.41  | 118.61      | 108.67   |
| 55  | 8     | 65   | ALA  | N-CA-C      | -6.38 | 105.66      | 113.50   |
| 48  | Z     | 66   | ARG  | N-CA-C      | -6.34 | 102.72      | 111.28   |
| 45  | W     | 66   | LEU  | N-CA-C      | -6.32 | 104.27      | 112.23   |
| 35  | M     | 126  | CYS  | N-CA-C      | 6.31  | 119.47      | 109.50   |
| 15  | r     | 55   | ASP  | N-CA-C      | 6.25  | 124.11      | 110.80   |
| 37  | O     | 40   | ILE  | CA-C-N      | 6.25  | 125.47      | 118.97   |
| 37  | O     | 40   | ILE  | C-N-CA      | 6.25  | 125.47      | 118.97   |
| 38  | P     | 47   | GLY  | N-CA-C      | -6.24 | 106.62      | 114.16   |
| 11  | n     | 68   | ALA  | N-CA-C      | -6.19 | 104.53      | 111.28   |
| 55  | 8     | 75   | GLN  | N-CA-C      | -6.16 | 105.26      | 112.89   |
| 38  | P     | 68   | ARG  | N-CA-C      | -6.15 | 104.68      | 111.82   |
| 7   | j     | 64   | VAL  | N-CA-C      | -6.13 | 99.85       | 108.80   |
| 9   | l     | 113  | ALA  | N-CA-C      | -6.13 | 103.21      | 112.04   |
| 55  | 8     | 37   | VAL  | N-CA-C      | -6.12 | 104.53      | 110.72   |
| 48  | Z     | 44   | ARG  | N-CA-C      | -6.12 | 104.53      | 111.14   |
| 43  | U     | 75   | ILE  | N-CA-C      | -6.08 | 104.58      | 110.72   |
| 3   | d     | 79   | ARG  | N-CA-C      | -6.07 | 101.48      | 110.46   |
| 38  | P     | 97   | ARG  | N-CA-C      | -6.07 | 104.58      | 112.23   |
| 51  | 1     | 1020 | A    | C2'-C3'-O3' | 6.05  | 118.58      | 109.50   |
| 49  | a     | 17   | ALA  | N-CA-C      | 6.05  | 118.84      | 111.82   |
| 33  | K     | 24   | ARG  | N-CA-C      | -6.04 | 104.27      | 111.69   |
| 35  | M     | 91   | LEU  | CA-C-N      | 6.02  | 126.22      | 119.90   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 35  | M     | 91  | LEU  | C-N-CA | 6.02  | 126.22      | 119.90   |
| 4   | e     | 171 | ALA  | N-CA-C | -6.00 | 104.85      | 111.82   |
| 4   | e     | 109 | ARG  | N-CA-C | -6.00 | 104.96      | 112.93   |
| 19  | v     | 40  | ILE  | N-CA-C | 6.00  | 117.23      | 108.53   |
| 42  | T     | 53  | ARG  | N-CA-C | -5.99 | 104.87      | 111.82   |
| 55  | 8     | 27  | TYR  | N-CA-C | 5.97  | 117.86      | 111.36   |
| 32  | J     | 131 | ASN  | CA-C-N | 5.95  | 127.28      | 119.84   |
| 32  | J     | 131 | ASN  | C-N-CA | 5.95  | 127.28      | 119.84   |
| 3   | d     | 31  | VAL  | N-CA-C | 5.94  | 116.12      | 110.42   |
| 32  | J     | 164 | LEU  | N-CA-C | -5.93 | 105.71      | 113.12   |
| 11  | n     | 67  | PHE  | N-CA-C | -5.91 | 106.20      | 113.41   |
| 30  | H     | 89  | VAL  | N-CA-C | 5.90  | 116.64      | 110.62   |
| 38  | P     | 90  | PRO  | N-CA-C | -5.90 | 106.31      | 114.27   |
| 20  | w     | 15  | LYS  | N-CA-C | 5.89  | 120.16      | 113.15   |
| 32  | J     | 81  | GLN  | N-CA-C | -5.88 | 106.64      | 113.88   |
| 47  | Y     | 85  | LEU  | N-CA-C | 5.88  | 119.55      | 112.38   |
| 29  | G     | 135 | MET  | N-CA-C | -5.88 | 104.96      | 111.36   |
| 55  | 8     | 109 | LYS  | N-CA-C | -5.86 | 105.97      | 113.23   |
| 55  | 8     | 288 | MET  | N-CA-C | -5.85 | 104.99      | 111.36   |
| 35  | M     | 72  | GLU  | N-CA-C | -5.79 | 104.60      | 111.03   |
| 8   | k     | 66  | LYS  | N-CA-C | -5.78 | 105.73      | 112.89   |
| 38  | P     | 100 | ASN  | N-CA-C | -5.77 | 104.96      | 112.23   |
| 18  | u     | 38  | ILE  | N-CA-C | -5.74 | 106.21      | 111.67   |
| 36  | N     | 89  | TYR  | N-CA-C | -5.74 | 103.86      | 111.96   |
| 33  | K     | 31  | GLY  | N-CA-C | -5.74 | 107.80      | 115.32   |
| 1   | b     | 145 | MET  | N-CA-C | -5.74 | 106.32      | 113.55   |
| 33  | K     | 76  | THR  | N-CA-C | -5.74 | 105.11      | 111.36   |
| 49  | a     | 191 | ALA  | N-CA-C | -5.73 | 105.17      | 111.82   |
| 1   | b     | 213 | ARG  | N-CA-C | -5.73 | 106.13      | 113.23   |
| 19  | v     | 48  | MET  | N-CA-C | -5.73 | 105.12      | 111.36   |
| 4   | e     | 69  | ALA  | N-CA-C | 5.71  | 118.50      | 110.23   |
| 47  | Y     | 39  | GLU  | N-CA-C | -5.70 | 105.15      | 111.36   |
| 1   | b     | 87  | SER  | N-CA-C | -5.68 | 106.70      | 113.97   |
| 10  | m     | 135 | VAL  | N-CA-C | 5.68  | 112.29      | 106.21   |
| 38  | P     | 54  | SER  | N-CA-C | -5.66 | 106.37      | 113.28   |
| 55  | 8     | 280 | GLN  | N-CA-C | 5.66  | 117.92      | 111.02   |
| 49  | a     | 56  | ASP  | N-CA-C | 5.63  | 118.19      | 111.71   |
| 15  | r     | 75  | VAL  | N-CA-C | 5.62  | 114.84      | 106.85   |
| 55  | 8     | 76  | GLY  | N-CA-C | -5.62 | 105.83      | 113.37   |
| 55  | 8     | 107 | GLU  | N-CA-C | -5.62 | 105.92      | 112.89   |
| 14  | q     | 24  | TYR  | N-CA-C | 5.59  | 118.35      | 109.24   |
| 55  | 8     | 17  | ARG  | N-CA-C | -5.59 | 106.47      | 113.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 47  | Y     | 48  | LYS  | N-CA-C | -5.57 | 105.13      | 111.14   |
| 49  | a     | 204 | ALA  | N-CA-C | 5.56  | 118.34      | 110.50   |
| 33  | K     | 40  | GLU  | N-CA-C | 5.54  | 117.50      | 108.63   |
| 28  | F     | 31  | PRO  | N-CA-C | -5.51 | 106.97      | 113.86   |
| 41  | S     | 92  | ILE  | N-CA-C | 5.50  | 113.93      | 107.77   |
| 2   | c     | 177 | VAL  | N-CA-C | -5.50 | 101.96      | 109.55   |
| 31  | I     | 89  | LEU  | N-CA-C | 5.49  | 117.69      | 111.11   |
| 6   | g     | 62  | LEU  | N-CA-C | -5.48 | 105.46      | 111.82   |
| 30  | H     | 18  | ASN  | N-CA-C | -5.48 | 105.64      | 112.93   |
| 32  | J     | 153 | ALA  | N-CA-C | -5.47 | 105.47      | 111.82   |
| 31  | I     | 166 | LYS  | CA-C-N | 5.46  | 126.67      | 119.84   |
| 31  | I     | 166 | LYS  | C-N-CA | 5.46  | 126.67      | 119.84   |
| 40  | R     | 110 | GLY  | CA-C-N | 5.45  | 125.46      | 119.90   |
| 40  | R     | 110 | GLY  | C-N-CA | 5.45  | 125.46      | 119.90   |
| 36  | N     | 91  | GLU  | N-CA-C | -5.44 | 105.74      | 112.38   |
| 35  | M     | 45  | ILE  | N-CA-C | -5.44 | 100.60      | 108.71   |
| 27  | E     | 61  | LEU  | CA-C-N | 5.44  | 124.95      | 119.19   |
| 27  | E     | 61  | LEU  | C-N-CA | 5.44  | 124.95      | 119.19   |
| 49  | a     | 28  | ALA  | N-CA-C | -5.44 | 105.51      | 111.82   |
| 48  | Z     | 11  | PHE  | N-CA-C | -5.44 | 105.34      | 112.41   |
| 40  | R     | 78  | ARG  | N-CA-C | -5.43 | 105.27      | 111.14   |
| 55  | 8     | 287 | ALA  | N-CA-C | -5.43 | 105.01      | 111.69   |
| 49  | a     | 6   | LYS  | N-CA-C | 5.43  | 120.28      | 111.37   |
| 34  | L     | 102 | TRP  | N-CA-C | 5.40  | 116.85      | 111.07   |
| 39  | Q     | 43  | LYS  | N-CA-C | 5.38  | 121.70      | 109.81   |
| 55  | 8     | 145 | ALA  | N-CA-C | -5.38 | 105.50      | 111.36   |
| 9   | l     | 26  | GLY  | N-CA-C | -5.37 | 107.83      | 115.30   |
| 34  | L     | 60  | ALA  | N-CA-C | -5.37 | 106.57      | 113.23   |
| 49  | a     | 193 | LEU  | N-CA-C | -5.37 | 105.09      | 111.69   |
| 1   | b     | 12  | ARG  | N-CA-C | -5.36 | 106.59      | 113.02   |
| 55  | 8     | 77  | LEU  | N-CA-C | -5.36 | 105.52      | 111.36   |
| 29  | G     | 5   | MET  | N-CA-C | 5.35  | 117.53      | 111.11   |
| 44  | V     | 66  | LEU  | N-CA-C | 5.35  | 118.03      | 111.82   |
| 31  | I     | 146 | GLU  | N-CA-C | 5.34  | 117.18      | 111.36   |
| 40  | R     | 80  | MET  | N-CA-C | -5.33 | 105.55      | 111.36   |
| 15  | r     | 14  | VAL  | N-CA-C | 5.31  | 116.37      | 108.46   |
| 12  | o     | 82  | ALA  | N-CA-C | -5.29 | 105.59      | 111.36   |
| 21  | x     | 68  | ALA  | N-CA-C | -5.29 | 105.59      | 111.36   |
| 4   | e     | 44  | ALA  | N-CA-C | -5.27 | 104.97      | 111.40   |
| 55  | 8     | 303 | LYS  | N-CA-C | -5.27 | 105.71      | 111.82   |
| 29  | G     | 196 | ASP  | N-CA-C | -5.26 | 106.92      | 113.55   |
| 14  | q     | 83  | LYS  | N-CA-C | -5.26 | 105.22      | 111.69   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26  | D     | 6    | GLN  | CA-C-N      | 5.25  | 125.26      | 119.90   |
| 26  | D     | 6    | GLN  | C-N-CA      | 5.25  | 125.26      | 119.90   |
| 3   | d     | 115  | GLN  | N-CA-C      | -5.25 | 106.90      | 113.72   |
| 28  | F     | 15   | LYS  | N-CA-C      | 5.24  | 117.83      | 110.23   |
| 38  | P     | 102  | ALA  | N-CA-C      | -5.24 | 105.75      | 111.82   |
| 3   | d     | 131  | THR  | N-CA-C      | 5.23  | 117.73      | 111.71   |
| 55  | 8     | 305  | ALA  | N-CA-C      | -5.23 | 105.75      | 111.82   |
| 48  | Z     | 9    | GLU  | N-CA-C      | 5.23  | 121.36      | 109.81   |
| 29  | G     | 46   | VAL  | CB-CA-C     | -5.22 | 108.74      | 113.70   |
| 55  | 8     | 230  | ILE  | N-CA-C      | 5.22  | 120.20      | 109.34   |
| 2   | c     | 150  | GLN  | N-CA-C      | 5.22  | 121.92      | 110.80   |
| 31  | I     | 111  | ALA  | N-CA-C      | -5.22 | 105.67      | 111.36   |
| 41  | S     | 16   | ALA  | N-CA-C      | -5.21 | 106.89      | 113.20   |
| 2   | c     | 152  | PRO  | N-CA-C      | -5.17 | 106.79      | 113.57   |
| 6   | g     | 63   | ALA  | N-CA-C      | -5.17 | 106.23      | 112.54   |
| 16  | s     | 52   | GLU  | N-CA-C      | -5.17 | 105.56      | 111.14   |
| 49  | a     | 192  | LEU  | N-CA-C      | -5.17 | 106.82      | 113.23   |
| 5   | f     | 109  | SER  | N-CA-C      | -5.15 | 107.37      | 113.97   |
| 49  | a     | 189  | LEU  | N-CA-C      | -5.15 | 106.50      | 112.89   |
| 50  | 3     | 1190 | G    | C2'-C3'-O3' | 5.14  | 117.22      | 109.50   |
| 34  | L     | 4    | ARG  | N-CA-C      | 5.14  | 117.75      | 110.10   |
| 4   | e     | 112  | ASP  | N-CA-C      | -5.13 | 105.86      | 111.82   |
| 30  | H     | 50   | SER  | N-CA-C      | 5.13  | 118.20      | 111.28   |
| 39  | Q     | 54   | VAL  | N-CA-C      | 5.12  | 115.10      | 108.35   |
| 1   | b     | 215  | VAL  | N-CA-C      | 5.11  | 115.27      | 108.11   |
| 3   | d     | 163  | ASN  | N-CA-C      | -5.11 | 108.79      | 114.62   |
| 30  | H     | 148  | ILE  | N-CA-C      | 5.11  | 115.26      | 108.11   |
| 29  | G     | 132  | GLU  | N-CA-C      | -5.11 | 105.79      | 111.36   |
| 40  | R     | 74   | MET  | N-CA-C      | -5.09 | 105.81      | 111.36   |
| 7   | j     | 45   | THR  | CA-C-N      | 5.09  | 125.38      | 119.47   |
| 7   | j     | 45   | THR  | C-N-CA      | 5.09  | 125.38      | 119.47   |
| 38  | P     | 63   | GLN  | N-CA-C      | -5.09 | 105.81      | 111.36   |
| 4   | e     | 164  | GLU  | N-CA-C      | -5.09 | 107.25      | 113.50   |
| 55  | 8     | 93   | GLU  | N-CA-C      | -5.09 | 107.08      | 113.28   |
| 19  | v     | 92   | VAL  | N-CA-C      | -5.08 | 102.95      | 109.30   |
| 55  | 8     | 41   | LEU  | N-CA-C      | -5.08 | 107.06      | 114.12   |
| 4   | e     | 11   | VAL  | N-CA-C      | 5.07  | 115.68      | 110.36   |
| 6   | g     | 51   | ARG  | N-CA-C      | 5.06  | 117.45      | 111.33   |
| 31  | I     | 78   | ALA  | N-CA-C      | -5.06 | 105.68      | 111.14   |
| 55  | 8     | 39   | ALA  | N-CA-C      | -5.05 | 105.86      | 112.23   |
| 11  | n     | 69   | ARG  | N-CA-C      | -5.05 | 102.59      | 110.42   |
| 30  | H     | 70   | ALA  | N-CA-C      | -5.05 | 107.78      | 114.04   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 55  | 8     | 353 | LEU  | N-CA-C | -5.05 | 107.29      | 113.50   |
| 14  | q     | 111 | LYS  | N-CA-C | -5.05 | 105.86      | 111.36   |
| 55  | 8     | 111 | ALA  | N-CA-C | -5.05 | 105.91      | 111.71   |
| 31  | I     | 173 | ASP  | N-CA-C | -5.04 | 104.78      | 112.04   |
| 45  | W     | 69  | TYR  | N-CA-C | -5.03 | 105.71      | 111.14   |
| 55  | 8     | 345 | THR  | N-CA-C | 5.03  | 119.67      | 111.37   |
| 29  | G     | 165 | ALA  | N-CA-C | 5.02  | 117.40      | 111.33   |
| 9   | l     | 17  | LYS  | N-CA-C | 5.02  | 116.66      | 108.63   |
| 42  | T     | 14  | PHE  | N-CA-C | -5.01 | 107.23      | 113.55   |
| 9   | l     | 95  | LEU  | N-CA-C | -5.01 | 106.34      | 112.90   |
| 3   | d     | 9   | GLN  | N-CA-C | 5.01  | 121.47      | 110.80   |
| 10  | m     | 107 | GLY  | N-CA-C | -5.01 | 108.09      | 114.85   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 2082  | 0        | 2157     | 106     | 0            |
| 2   | c     | 1565  | 0        | 1616     | 85      | 0            |
| 3   | d     | 1552  | 0        | 1619     | 91      | 0            |
| 4   | e     | 1410  | 0        | 1447     | 101     | 0            |
| 5   | f     | 1323  | 0        | 1374     | 83      | 0            |
| 6   | g     | 1111  | 0        | 1148     | 86      | 0            |
| 7   | j     | 1129  | 0        | 1162     | 52      | 0            |
| 8   | k     | 938   | 0        | 1012     | 39      | 0            |
| 9   | l     | 1045  | 0        | 1117     | 52      | 0            |
| 10  | m     | 1074  | 0        | 1157     | 62      | 0            |
| 11  | n     | 960   | 0        | 1000     | 36      | 0            |
| 12  | o     | 892   | 0        | 923      | 52      | 0            |
| 13  | p     | 917   | 0        | 965      | 61      | 0            |
| 14  | q     | 947   | 0        | 1022     | 49      | 0            |
| 15  | r     | 816   | 0        | 839      | 54      | 0            |
| 16  | s     | 857   | 0        | 922      | 39      | 0            |
| 17  | t     | 738   | 0        | 807      | 37      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 18  | u     | 779    | 0        | 834      | 38      | 0            |
| 19  | v     | 753    | 0        | 780      | 33      | 0            |
| 20  | w     | 575    | 0        | 592      | 19      | 0            |
| 21  | x     | 625    | 0        | 655      | 29      | 0            |
| 22  | y     | 509    | 0        | 543      | 19      | 0            |
| 23  | z     | 449    | 0        | 491      | 14      | 0            |
| 24  | B     | 444    | 0        | 461      | 23      | 0            |
| 25  | C     | 409    | 0        | 440      | 23      | 0            |
| 26  | D     | 377    | 0        | 418      | 17      | 0            |
| 27  | E     | 504    | 0        | 574      | 28      | 0            |
| 28  | F     | 302    | 0        | 343      | 18      | 0            |
| 29  | G     | 1756   | 0        | 1787     | 102     | 0            |
| 30  | H     | 1624   | 0        | 1699     | 96      | 0            |
| 31  | I     | 1643   | 0        | 1710     | 102     | 0            |
| 32  | J     | 1156   | 0        | 1199     | 80      | 0            |
| 33  | K     | 824    | 0        | 815      | 77      | 0            |
| 34  | L     | 1181   | 0        | 1240     | 79      | 0            |
| 35  | M     | 979    | 0        | 1034     | 58      | 0            |
| 36  | N     | 1022   | 0        | 1070     | 86      | 0            |
| 37  | O     | 786    | 0        | 828      | 59      | 0            |
| 38  | P     | 869    | 0        | 878      | 71      | 0            |
| 39  | Q     | 955    | 0        | 1019     | 75      | 0            |
| 40  | R     | 883    | 0        | 944      | 66      | 0            |
| 41  | S     | 805    | 0        | 847      | 73      | 0            |
| 42  | T     | 714    | 0        | 737      | 34      | 0            |
| 43  | U     | 649    | 0        | 666      | 48      | 0            |
| 44  | V     | 648    | 0        | 691      | 35      | 0            |
| 45  | W     | 535    | 0        | 552      | 25      | 0            |
| 46  | X     | 637    | 0        | 665      | 54      | 0            |
| 47  | Y     | 665    | 0        | 714      | 39      | 0            |
| 48  | Z     | 544    | 0        | 579      | 47      | 0            |
| 49  | a     | 1026   | 0        | 1092     | 60      | 0            |
| 50  | 3     | 33012  | 0        | 16618    | 617     | 0            |
| 51  | 1     | 62317  | 0        | 31346    | 1008    | 0            |
| 52  | 2     | 2568   | 0        | 1303     | 66      | 0            |
| 53  | 5     | 1556   | 0        | 793      | 20      | 0            |
| 54  | 4     | 437    | 0        | 219      | 12      | 0            |
| 55  | 8     | 2860   | 0        | 2758     | 168     | 0            |
| All | All   | 147733 | 0        | 100221   | 3994    | 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 16.

All (3994) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:J:55:VAL:HG23  | 32:J:56:PRO:HD3   | 1.24                     | 1.13              |
| 51:1:2800:A:H3'   | 51:1:2801:G:H5'   | 1.36                     | 1.06              |
| 34:L:111:GLY:HA2  | 34:L:118:ARG:HD3  | 1.33                     | 1.04              |
| 51:1:1645:G:H5''  | 51:1:1646:C:H5'   | 1.35                     | 1.03              |
| 51:1:2747:G:H2'   | 51:1:2748:A:H5''  | 1.41                     | 1.01              |
| 40:R:25:GLY:H     | 50:3:1329:A:H5''  | 1.23                     | 1.00              |
| 51:1:2244:U:H3'   | 51:1:2245:U:H5''  | 1.41                     | 1.00              |
| 51:1:1270:C:H5''  | 51:1:1271:G:H5''  | 1.41                     | 0.99              |
| 37:O:7:ARG:HB3    | 37:O:101:SER:HB3  | 1.43                     | 0.99              |
| 15:r:6:GLN:HG3    | 15:r:11:GLN:HE22  | 1.26                     | 0.98              |
| 21:x:5:GLN:HG3    | 21:x:49:ARG:HB2   | 1.45                     | 0.98              |
| 40:R:15:VAL:HG23  | 40:R:16:ILE:HD12  | 1.45                     | 0.98              |
| 34:L:90:VAL:HG13  | 34:L:95:ARG:HG2   | 1.42                     | 0.97              |
| 36:N:20:ILE:HD11  | 36:N:60:LEU:HD13  | 1.44                     | 0.97              |
| 50:3:279:A:H5'    | 50:3:281:G:H5'    | 1.46                     | 0.97              |
| 43:U:31:ARG:HB2   | 50:3:310:G:H5''   | 1.45                     | 0.97              |
| 6:g:132:PHE:HB2   | 6:g:140:ALA:HB3   | 1.47                     | 0.96              |
| 8:k:105:ARG:HD3   | 8:k:108:ARG:HH22  | 1.29                     | 0.96              |
| 39:Q:97:VAL:HG23  | 39:Q:100:ALA:HB2  | 1.43                     | 0.96              |
| 55:8:21:LEU:HD22  | 55:8:113:LEU:HG   | 1.45                     | 0.96              |
| 27:E:18:LYS:HG3   | 51:1:651:G:H5'    | 1.45                     | 0.95              |
| 53:5:15:G:H22     | 53:5:48:C:H42     | 1.08                     | 0.95              |
| 44:V:57:VAL:HG13  | 44:V:78:VAL:HG23  | 1.49                     | 0.94              |
| 51:1:1527:G:H21   | 51:1:1545:A:H62   | 1.17                     | 0.93              |
| 1:b:106:PRO:HD2   | 1:b:109:LEU:HD22  | 1.50                     | 0.93              |
| 49:a:205:LYS:HA   | 51:1:1860:G:H4'   | 1.50                     | 0.93              |
| 51:1:1179:G:H2'   | 51:1:1180:U:H4'   | 1.51                     | 0.93              |
| 14:q:107:ALA:HB3  | 15:r:48:LYS:NZ    | 1.82                     | 0.93              |
| 30:H:151:GLU:HG3  | 30:H:166:TRP:HB3  | 1.49                     | 0.92              |
| 51:1:2277:G:H2'   | 51:1:2278:A:H5''  | 1.51                     | 0.92              |
| 51:1:2063:C:H4'   | 55:8:251:GLY:HA3  | 1.52                     | 0.91              |
| 4:e:147:ARG:HB3   | 4:e:149:ARG:HE    | 1.34                     | 0.91              |
| 34:L:35:LYS:HE2   | 50:3:1373:G:H5''  | 1.48                     | 0.91              |
| 13:p:24:THR:HG23  | 13:p:86:LYS:HB2   | 1.51                     | 0.90              |
| 55:8:120:SER:HB3  | 55:8:193:ARG:HH21 | 1.34                     | 0.90              |
| 14:q:107:ALA:HB3  | 15:r:48:LYS:HZ2   | 1.36                     | 0.90              |
| 33:K:47:LEU:H     | 33:K:55:HIS:HB3   | 1.37                     | 0.89              |
| 55:8:323:ILE:HG23 | 55:8:337:ARG:HD2  | 1.52                     | 0.89              |
| 15:r:27:ILE:HG23  | 15:r:28:ALA:H     | 1.36                     | 0.89              |
| 25:C:22:THR:HG22  | 25:C:23:THR:H     | 1.37                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:8:348:VAL:HA   | 55:8:352:SER:HB3  | 1.53                     | 0.89              |
| 26:D:11:LYS:HE2   | 51:1:686:U:H5''   | 1.54                     | 0.88              |
| 34:L:49:LEU:HD22  | 34:L:123:LEU:HD13 | 1.53                     | 0.88              |
| 36:N:51:LEU:HD13  | 36:N:56:MET:HG3   | 1.56                     | 0.88              |
| 51:1:783:A:H2'    | 51:1:784:G:H4'    | 1.54                     | 0.87              |
| 13:p:59:THR:HG22  | 13:p:72:VAL:HG12  | 1.57                     | 0.87              |
| 51:1:1103:A:H3'   | 51:1:1104:C:H5''  | 1.57                     | 0.87              |
| 55:8:18:SER:HB2   | 55:8:70:LEU:HD13  | 1.56                     | 0.87              |
| 55:8:266:ILE:HG13 | 55:8:267:PRO:HD3  | 1.56                     | 0.87              |
| 33:K:23:GLU:HA    | 33:K:26:THR:HG22  | 1.55                     | 0.87              |
| 31:I:25:ARG:NH1   | 31:I:25:ARG:HB2   | 1.90                     | 0.86              |
| 49:a:5:THR:HG22   | 49:a:6:LYS:H      | 1.39                     | 0.86              |
| 50:3:993:G:H21    | 50:3:996:A:H61    | 1.19                     | 0.86              |
| 2:c:116:LYS:HA    | 11:n:1:MET:HE1    | 1.55                     | 0.86              |
| 37:O:31:ARG:HD2   | 37:O:32:THR:HG23  | 1.58                     | 0.86              |
| 41:S:29:ILE:HG13  | 41:S:30:ILE:HD12  | 1.55                     | 0.86              |
| 10:m:45:GLN:HE21  | 51:1:2485:G:H5''  | 1.38                     | 0.86              |
| 50:3:327:A:O2'    | 50:3:328:C:H4'    | 1.73                     | 0.86              |
| 48:Z:33:ARG:HH21  | 48:Z:34:ARG:HD2   | 1.40                     | 0.86              |
| 51:1:548:G:H2'    | 51:1:549:G:H4'    | 1.56                     | 0.85              |
| 46:X:80:ARG:HG2   | 50:3:956:U:H4'    | 1.58                     | 0.85              |
| 40:R:13:HIS:HB2   | 40:R:16:ILE:HD13  | 1.59                     | 0.85              |
| 23:z:6:ILE:HG22   | 23:z:56:VAL:HG12  | 1.57                     | 0.84              |
| 49:a:215:SER:HB2  | 51:1:2176:A:H1'   | 1.60                     | 0.83              |
| 4:e:32:LYS:HB3    | 4:e:156:THR:HB    | 1.60                     | 0.83              |
| 29:G:42:LEU:HD23  | 29:G:42:LEU:H     | 1.43                     | 0.83              |
| 49:a:24:ASN:HB3   | 49:a:186:LYS:HG3  | 1.60                     | 0.83              |
| 50:3:167:A:H3'    | 50:3:168:G:H5''   | 1.59                     | 0.83              |
| 51:1:1020:A:H1'   | 51:1:1021:A:OP2   | 1.78                     | 0.83              |
| 19:v:49:ASN:OD1   | 51:1:1040:A:H4'   | 1.77                     | 0.83              |
| 31:I:25:ARG:HB2   | 31:I:25:ARG:HH11  | 1.44                     | 0.83              |
| 51:1:1141:U:H4'   | 51:1:1142:A:O4'   | 1.79                     | 0.83              |
| 5:f:173:ALA:HA    | 51:1:2531:A:O4'   | 1.78                     | 0.83              |
| 15:r:14:VAL:HG11  | 15:r:98:ILE:HG13  | 1.61                     | 0.83              |
| 5:f:16:VAL:HG21   | 5:f:49:LEU:HD11   | 1.60                     | 0.83              |
| 50:3:516:U:H3     | 50:3:533:A:H62    | 1.24                     | 0.83              |
| 39:Q:72:ASN:ND2   | 39:Q:98:ARG:HE    | 1.77                     | 0.82              |
| 43:U:54:LEU:HD22  | 43:U:80:LYS:HE2   | 1.61                     | 0.82              |
| 2:c:148:GLN:HB2   | 2:c:152:PRO:HG2   | 1.61                     | 0.82              |
| 6:g:66:ASN:O      | 6:g:70:GLU:HG3    | 1.79                     | 0.82              |
| 26:D:24:THR:HG23  | 26:D:27:GLY:H     | 1.44                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:1:2747:G:C2'   | 51:1:2748:A:H5''  | 2.09                     | 0.82              |
| 49:a:48:LEU:HD21  | 49:a:171:ILE:HD11 | 1.61                     | 0.82              |
| 30:H:4:VAL:HG23   | 30:H:5:HIS:H      | 1.44                     | 0.82              |
| 34:L:72:VAL:HG21  | 34:L:144:ALA:HB2  | 1.62                     | 0.82              |
| 49:a:11:ILE:HG23  | 49:a:33:LEU:HD22  | 1.61                     | 0.81              |
| 34:L:62:GLU:O     | 34:L:66:GLU:HG2   | 1.81                     | 0.81              |
| 41:S:79:SER:HB3   | 41:S:82:LYS:HG2   | 1.62                     | 0.81              |
| 50:3:484:G:H4'    | 50:3:485:U:H5''   | 1.62                     | 0.81              |
| 51:1:1415:U:H2'   | 51:1:1416:G:H4'   | 1.63                     | 0.81              |
| 50:3:405:U:H3'    | 50:3:406:G:H5'    | 1.61                     | 0.81              |
| 51:1:215:G:H4'    | 51:1:216:A:H4'    | 1.61                     | 0.81              |
| 51:1:2629:U:H4'   | 51:1:2630:G:H5''  | 1.61                     | 0.81              |
| 33:K:12:PRO:HB3   | 33:K:44:ARG:HH11  | 1.44                     | 0.81              |
| 33:K:71:ILE:HD11  | 33:K:89:VAL:HG21  | 1.62                     | 0.81              |
| 35:M:9:MET:HG3    | 35:M:26:MET:SD    | 2.21                     | 0.81              |
| 24:B:31:LYS:HE3   | 51:1:2885:G:H1    | 1.44                     | 0.81              |
| 39:Q:23:LEU:HD23  | 39:Q:26:CYS:SG    | 2.20                     | 0.81              |
| 12:o:63:LYS:NZ    | 52:2:51:G:H5'     | 1.96                     | 0.80              |
| 47:Y:70:LYS:HA    | 47:Y:73:ARG:NH1   | 1.96                     | 0.80              |
| 10:m:35:ALA:HB2   | 10:m:102:LEU:HD11 | 1.62                     | 0.80              |
| 42:T:48:ASP:HB3   | 42:T:51:SER:OG    | 1.81                     | 0.80              |
| 35:M:88:LYS:HD3   | 50:3:600:A:H5''   | 1.62                     | 0.80              |
| 51:1:1073:A:H2'   | 51:1:1074:G:H5'   | 1.63                     | 0.80              |
| 53:5:26:G:H1      | 53:5:44:A:H61     | 1.27                     | 0.80              |
| 18:u:65:GLN:HG2   | 51:1:328:U:H4'    | 1.64                     | 0.80              |
| 30:H:112:ALA:HB3  | 30:H:184:ASN:HD22 | 1.46                     | 0.80              |
| 6:g:97:ARG:HH21   | 6:g:100:ALA:HB1   | 1.44                     | 0.80              |
| 6:g:89:LYS:H      | 6:g:124:THR:HG23  | 1.46                     | 0.79              |
| 2:c:179:ARG:HH11  | 2:c:188:LEU:HD12  | 1.47                     | 0.79              |
| 33:K:9:MET:HB3    | 33:K:57:ALA:HB1   | 1.63                     | 0.79              |
| 34:L:132:THR:HA   | 34:L:135:LYS:HD2  | 1.63                     | 0.79              |
| 36:N:17:ARG:HB2   | 36:N:65:THR:HB    | 1.64                     | 0.79              |
| 24:B:39:ARG:HG3   | 24:B:40:HIS:ND1   | 1.96                     | 0.79              |
| 16:s:42:LYS:HB2   | 51:1:2010:G:H5''  | 1.62                     | 0.79              |
| 51:1:2747:G:H21   | 51:1:2757:A:H62   | 1.30                     | 0.79              |
| 9:l:92:LEU:HD23   | 9:l:92:LEU:H      | 1.47                     | 0.78              |
| 16:s:93:ALA:HB2   | 51:1:1614:A:N1    | 1.97                     | 0.78              |
| 2:c:151:THR:HB    | 2:c:152:PRO:HD3   | 1.64                     | 0.78              |
| 35:M:28:SER:HB2   | 35:M:56:PRO:HB2   | 1.66                     | 0.78              |
| 36:N:105:ARG:HG2  | 50:3:1117:A:O3'   | 1.84                     | 0.78              |
| 30:H:156:LEU:HD21 | 30:H:163:ARG:HB2  | 1.64                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:1:1668:A:H4'   | 51:1:1669:A:H5'   | 1.66                     | 0.78              |
| 55:8:17:ARG:HH21  | 55:8:362:LYS:HD3  | 1.49                     | 0.78              |
| 5:f:137:LYS:HD2   | 51:1:2746:U:H5''  | 1.66                     | 0.78              |
| 4:e:57:ALA:HB2    | 4:e:64:PRO:HD3    | 1.64                     | 0.78              |
| 8:k:121:GLU:HG3   | 8:k:122:VAL:HG23  | 1.66                     | 0.78              |
| 31:I:154:VAL:HG11 | 31:I:177:MET:HE3  | 1.64                     | 0.78              |
| 15:r:49:ILE:HG22  | 15:r:54:VAL:HG13  | 1.64                     | 0.78              |
| 38:P:87:GLY:H     | 38:P:113:THR:HG22 | 1.49                     | 0.78              |
| 51:1:1912:A:H62   | 51:1:1917:U:H3    | 1.31                     | 0.78              |
| 6:g:134:VAL:HG23  | 6:g:138:VAL:HG13  | 1.66                     | 0.78              |
| 37:O:52:LEU:HD11  | 41:S:80:ARG:HH21  | 1.49                     | 0.78              |
| 6:g:31:VAL:HG23   | 6:g:32:PRO:HD3    | 1.64                     | 0.77              |
| 21:x:31:ASN:HD22  | 21:x:52:ALA:HB2   | 1.49                     | 0.77              |
| 50:3:211:G:H2'    | 50:3:212:G:H5'    | 1.66                     | 0.77              |
| 6:g:103:VAL:HG12  | 6:g:108:VAL:HB    | 1.65                     | 0.77              |
| 10:m:45:GLN:NE2   | 51:1:2485:G:H5''  | 2.00                     | 0.77              |
| 39:Q:72:ASN:HD21  | 39:Q:98:ARG:HE    | 1.31                     | 0.77              |
| 41:S:40:ARG:HH22  | 46:X:6:LYS:HB3    | 1.49                     | 0.77              |
| 44:V:30:HIS:HB2   | 44:V:37:ILE:HD11  | 1.65                     | 0.77              |
| 32:J:10:LEU:HD23  | 32:J:10:LEU:H     | 1.48                     | 0.77              |
| 47:Y:66:ILE:HD12  | 47:Y:70:LYS:HZ2   | 1.50                     | 0.77              |
| 51:1:2573:C:H42   | 55:8:257:THR:HG21 | 1.49                     | 0.77              |
| 1:b:209:ALA:HA    | 1:b:212:TRP:NE1   | 2.00                     | 0.76              |
| 10:m:42:THR:OG1   | 10:m:45:GLN:HG3   | 1.85                     | 0.76              |
| 48:Z:11:PHE:HA    | 48:Z:15:LEU:HD22  | 1.67                     | 0.76              |
| 4:e:38:GLY:HA3    | 51:1:2312:U:H1'   | 1.65                     | 0.76              |
| 35:M:14:ARG:HG3   | 35:M:74:ILE:HG22  | 1.65                     | 0.76              |
| 40:R:25:GLY:N     | 50:3:1329:A:H5''  | 1.98                     | 0.76              |
| 49:a:30:LEU:HD21  | 49:a:42:VAL:HG21  | 1.66                     | 0.76              |
| 39:Q:23:LEU:HD22  | 39:Q:29:LYS:NZ    | 1.99                     | 0.76              |
| 5:f:159:LYS:HE3   | 51:1:2658:C:H5''  | 1.67                     | 0.76              |
| 46:X:54:ARG:HG3   | 46:X:55:GLN:HG3   | 1.67                     | 0.76              |
| 51:1:774:G:O2'    | 51:1:775:G:H5''   | 1.85                     | 0.76              |
| 24:B:31:LYS:HE3   | 51:1:2885:G:N1    | 1.99                     | 0.76              |
| 51:1:2277:G:C2'   | 51:1:2278:A:H5''  | 2.16                     | 0.76              |
| 9:l:54:GLN:HE22   | 51:1:2358:A:H61   | 1.34                     | 0.76              |
| 30:H:2:GLN:HB2    | 50:3:1190:G:O3'   | 1.86                     | 0.76              |
| 36:N:69:GLY:N     | 50:3:1250:A:H4'   | 2.01                     | 0.76              |
| 48:Z:23:GLU:CD    | 48:Z:24:LYS:H     | 1.94                     | 0.76              |
| 3:d:146:VAL:HG12  | 3:d:185:LYS:HB2   | 1.66                     | 0.75              |
| 46:X:59:VAL:HG11  | 46:X:70:LEU:HD11  | 1.68                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:1:1043:C:H2'   | 51:1:1044:C:H5'   | 1.67                     | 0.75              |
| 37:O:47:GLU:HB2   | 37:O:67:ILE:HB    | 1.66                     | 0.75              |
| 38:P:88:PRO:HG3   | 48:Z:28:LEU:HD21  | 1.69                     | 0.75              |
| 45:W:33:THR:HG22  | 45:W:37:LYS:H     | 1.50                     | 0.75              |
| 51:1:511:U:H2'    | 51:1:512:G:H5'    | 1.68                     | 0.75              |
| 5:f:19:ASN:OD1    | 5:f:22:VAL:HG23   | 1.86                     | 0.75              |
| 30:H:112:ALA:HB2  | 30:H:182:ASP:HB3  | 1.69                     | 0.75              |
| 15:r:4:VAL:HG13   | 15:r:39:LEU:HB3   | 1.69                     | 0.74              |
| 37:O:10:LEU:HD23  | 37:O:10:LEU:H     | 1.52                     | 0.74              |
| 20:w:38:GLY:HA2   | 51:1:2330:G:H21   | 1.50                     | 0.74              |
| 50:3:225:C:H3'    | 50:3:226:G:H5''   | 1.69                     | 0.74              |
| 50:3:1239:A:H62   | 50:3:1299:A:H2    | 1.34                     | 0.74              |
| 51:1:310:A:O2'    | 51:1:311:A:H2'    | 1.88                     | 0.74              |
| 51:1:2287:A:H61   | 51:1:2344:U:H3    | 1.34                     | 0.74              |
| 34:L:74:VAL:HB    | 34:L:85:GLN:HB3   | 1.68                     | 0.74              |
| 36:N:123:ARG:HB2  | 50:3:1343:G:H4'   | 1.69                     | 0.74              |
| 8:k:18:ARG:HB3    | 8:k:45:GLU:HB2    | 1.68                     | 0.74              |
| 46:X:10:ILE:HG13  | 46:X:11:ASP:H     | 1.53                     | 0.74              |
| 49:a:23:ILE:HD11  | 49:a:189:LEU:HD13 | 1.69                     | 0.74              |
| 51:1:2440:C:H2'   | 51:1:2441:U:H4'   | 1.69                     | 0.74              |
| 11:n:38:LEU:HB3   | 11:n:39:PRO:HD3   | 1.69                     | 0.74              |
| 36:N:51:LEU:HD22  | 36:N:56:MET:HB2   | 1.68                     | 0.74              |
| 38:P:27:ASN:HB3   | 38:P:56:LYS:HZ1   | 1.53                     | 0.74              |
| 50:3:1158:C:H2'   | 50:3:1159:U:H4'   | 1.70                     | 0.74              |
| 3:d:5:LEU:HD22    | 3:d:10:SER:HB2    | 1.69                     | 0.74              |
| 15:r:76:LYS:HB2   | 15:r:85:LYS:HB3   | 1.69                     | 0.74              |
| 41:S:74:ARG:NH2   | 50:3:1359:C:H3'   | 2.03                     | 0.74              |
| 43:U:5:ARG:HB2    | 50:3:376:G:H5''   | 1.70                     | 0.74              |
| 51:1:876:C:H2'    | 51:1:877:A:H5'    | 1.70                     | 0.74              |
| 51:1:1073:A:H61   | 55:8:54:GLN:HG3   | 1.53                     | 0.73              |
| 6:g:65:ALA:HA     | 6:g:68:ARG:HE     | 1.52                     | 0.73              |
| 34:L:58:LEU:H     | 34:L:58:LEU:HD12  | 1.53                     | 0.73              |
| 8:k:49:ARG:HH22   | 50:3:1422:G:H4'   | 1.53                     | 0.73              |
| 9:l:95:LEU:HG     | 9:l:100:ILE:HD11  | 1.68                     | 0.73              |
| 10:m:3:GLN:HE21   | 10:m:92:TRP:HE1   | 1.36                     | 0.73              |
| 51:1:1367:A:H2'   | 51:1:1368:G:H5'   | 1.68                     | 0.73              |
| 55:8:333:ILE:HG13 | 55:8:345:THR:HG22 | 1.69                     | 0.73              |
| 31:I:114:ARG:NH1  | 31:I:132:ALA:HB3  | 2.02                     | 0.73              |
| 37:O:58:ASN:ND2   | 50:3:1061:G:H4'   | 2.04                     | 0.73              |
| 27:E:3:ILE:HD12   | 27:E:62:PRO:HG2   | 1.71                     | 0.73              |
| 50:3:959:A:H2'    | 50:3:960:U:H4'    | 1.70                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:3:1069:C:H41   | 50:3:1094:G:H1    | 1.36                     | 0.73              |
| 29:G:198:VAL:C    | 29:G:199:ILE:HD12 | 2.13                     | 0.73              |
| 30:H:156:LEU:HD11 | 30:H:163:ARG:HD3  | 1.69                     | 0.73              |
| 35:M:121:GLY:C    | 50:3:599:C:H4'    | 2.13                     | 0.73              |
| 47:Y:42:ASP:HB2   | 47:Y:45:ALA:HB3   | 1.68                     | 0.73              |
| 50:3:78:A:H61     | 50:3:91:U:H3      | 1.37                     | 0.73              |
| 1:b:152:GLN:HG3   | 51:1:1818:U:O4    | 1.89                     | 0.73              |
| 11:n:44:LEU:HD23  | 11:n:113:ILE:HD13 | 1.70                     | 0.73              |
| 13:p:101:GLU:OE2  | 13:p:102:ARG:HG3  | 1.87                     | 0.73              |
| 29:G:101:THR:HG23 | 50:3:1074:G:H4'   | 1.70                     | 0.73              |
| 30:H:182:ASP:HB2  | 30:H:201:ILE:HB   | 1.70                     | 0.73              |
| 33:K:37:HIS:HB3   | 33:K:97:THR:HG22  | 1.71                     | 0.73              |
| 52:2:3:C:H2'      | 52:2:4:C:H5''     | 1.70                     | 0.73              |
| 52:2:12:C:O2'     | 52:2:13:G:H4'     | 1.89                     | 0.73              |
| 51:1:615:U:H5''   | 51:1:616:A:OP2    | 1.89                     | 0.73              |
| 33:K:17:GLN:O     | 33:K:21:MET:HE3   | 1.89                     | 0.73              |
| 41:S:52:ARG:HH21  | 50:3:1015:G:H5'   | 1.54                     | 0.72              |
| 51:1:940:G:H2'    | 51:1:941:A:H5''   | 1.71                     | 0.72              |
| 51:1:1807:G:H2'   | 51:1:1808:A:H5'   | 1.71                     | 0.72              |
| 52:2:3:C:C3'      | 52:2:4:C:H5''     | 2.19                     | 0.72              |
| 13:p:4:ILE:H      | 13:p:4:ILE:HD12   | 1.54                     | 0.72              |
| 50:3:1166:G:H21   | 50:3:1170:A:H62   | 1.36                     | 0.72              |
| 51:1:2629:U:H5''  | 51:1:2630:G:OP1   | 1.90                     | 0.72              |
| 4:e:45:ASP:OD1    | 4:e:47:LYS:HG2    | 1.89                     | 0.72              |
| 43:U:20:VAL:HG23  | 43:U:34:GLU:O     | 1.89                     | 0.72              |
| 55:8:15:THR:HG21  | 55:8:77:LEU:HD22  | 1.70                     | 0.72              |
| 3:d:69:ARG:HH12   | 51:1:2060:A:N6    | 1.88                     | 0.72              |
| 10:m:135:VAL:HG12 | 19:v:79:ARG:HH22  | 1.54                     | 0.72              |
| 2:c:4:LEU:HD22    | 2:c:101:PHE:CE2   | 2.23                     | 0.72              |
| 1:b:257:ARG:HB2   | 51:1:1798:U:OP1   | 1.89                     | 0.72              |
| 3:d:48:THR:HG22   | 3:d:51:GLU:HG3    | 1.70                     | 0.72              |
| 6:g:93:SER:HB3    | 6:g:121:VAL:HG21  | 1.71                     | 0.72              |
| 34:L:46:LEU:HB3   | 34:L:57:GLU:OE2   | 1.90                     | 0.72              |
| 36:N:45:MET:HB3   | 36:N:48:ARG:HH21  | 1.54                     | 0.72              |
| 14:q:87:VAL:HG13  | 15:r:49:ILE:HD11  | 1.71                     | 0.71              |
| 33:K:18:VAL:N     | 33:K:19:PRO:HD3   | 2.04                     | 0.71              |
| 2:c:40:LEU:H      | 2:c:40:LEU:HD12   | 1.54                     | 0.71              |
| 5:f:18:ILE:HD12   | 5:f:44:HIS:HB2    | 1.72                     | 0.71              |
| 12:o:76:LYS:O     | 12:o:80:GLU:HG3   | 1.90                     | 0.71              |
| 50:3:167:A:C3'    | 50:3:168:G:H5''   | 2.18                     | 0.71              |
| 29:G:161:PHE:HA   | 29:G:183:PHE:HB2  | 1.73                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:H:168:ARG:HH21 | 30:H:172:VAL:HB   | 1.55                     | 0.71              |
| 51:1:1168:G:H1    | 51:1:1181:U:H3    | 1.35                     | 0.71              |
| 1:b:220:ARG:HH22  | 1:b:237:ARG:HH21  | 1.38                     | 0.71              |
| 21:x:60:LYS:HG2   | 51:1:372:G:O4'    | 1.91                     | 0.71              |
| 30:H:85:LYS:HA    | 30:H:88:LYS:HD3   | 1.71                     | 0.71              |
| 5:f:21:GLN:HE22   | 5:f:38:ASP:HA     | 1.54                     | 0.71              |
| 30:H:111:ASP:OD2  | 30:H:114:LEU:HD23 | 1.90                     | 0.71              |
| 55:8:144:TRP:CG   | 55:8:201:LEU:HD22 | 2.24                     | 0.71              |
| 1:b:94:LEU:HD13   | 1:b:100:ARG:HG2   | 1.72                     | 0.71              |
| 24:B:37:HIS:HB3   | 24:B:43:THR:HG22  | 1.73                     | 0.71              |
| 4:e:109:ARG:HD3   | 4:e:136:ILE:HA    | 1.72                     | 0.71              |
| 15:r:6:GLN:HG3    | 15:r:11:GLN:NE2   | 2.04                     | 0.71              |
| 52:2:3:C:H3'      | 52:2:4:C:H5''     | 1.72                     | 0.71              |
| 8:k:76:VAL:H      | 13:p:72:VAL:HG22  | 1.56                     | 0.71              |
| 12:o:63:LYS:HZ1   | 52:2:51:G:H5'     | 1.52                     | 0.71              |
| 2:c:56:LYS:HB2    | 2:c:59:ARG:HB2    | 1.71                     | 0.71              |
| 10:m:53:MET:HE1   | 10:m:117:PHE:HA   | 1.72                     | 0.71              |
| 5:f:17:LYS:HE2    | 5:f:17:LYS:HA     | 1.71                     | 0.70              |
| 31:I:131:ILE:H    | 31:I:131:ILE:HD12 | 1.55                     | 0.70              |
| 50:3:346:G:H2'    | 50:3:347:G:H5'    | 1.72                     | 0.70              |
| 51:1:917:A:H5''   | 51:1:2268:A:H61   | 1.54                     | 0.70              |
| 53:5:6:G:O2'      | 53:5:7:G:H5'      | 1.91                     | 0.70              |
| 36:N:69:GLY:H     | 50:3:1250:A:H4'   | 1.56                     | 0.70              |
| 29:G:94:ARG:HH22  | 50:3:1102:A:H4'   | 1.55                     | 0.70              |
| 55:8:297:GLU:HA   | 55:8:300:MET:HE2  | 1.71                     | 0.70              |
| 55:8:342:THR:HG22 | 55:8:344:ASN:H    | 1.56                     | 0.70              |
| 27:E:57:VAL:O     | 27:E:61:LEU:HD23  | 1.92                     | 0.70              |
| 36:N:129:ARG:HD2  | 36:N:129:ARG:N    | 2.05                     | 0.70              |
| 43:U:70:ARG:HE    | 43:U:74:LEU:HD21  | 1.56                     | 0.70              |
| 55:8:166:ILE:HB   | 55:8:180:THR:HG23 | 1.73                     | 0.70              |
| 14:q:23:TYR:CD1   | 51:1:533:G:H5'    | 2.27                     | 0.70              |
| 31:I:114:ARG:HH11 | 31:I:132:ALA:HB3  | 1.56                     | 0.70              |
| 13:p:85:VAL:HG11  | 13:p:88:ARG:NH2   | 2.07                     | 0.70              |
| 18:u:37:GLY:HA2   | 18:u:61:GLU:HG2   | 1.73                     | 0.70              |
| 30:H:151:GLU:CG   | 30:H:166:TRP:HB3  | 2.22                     | 0.70              |
| 38:P:33:ILE:HD12  | 38:P:73:VAL:HG11  | 1.72                     | 0.70              |
| 42:T:55:LEU:O     | 42:T:59:VAL:HG23  | 1.92                     | 0.70              |
| 9:l:79:LEU:HB2    | 9:l:114:GLY:H     | 1.57                     | 0.70              |
| 50:3:1346:A:O2'   | 50:3:1347:G:H4'   | 1.92                     | 0.70              |
| 51:1:2313:C:O2'   | 51:1:2314:A:H5'   | 1.92                     | 0.70              |
| 55:8:130:LEU:HD11 | 55:8:192:LEU:HD13 | 1.74                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:d:3:LEU:HD11    | 3:d:14:VAL:HG11   | 1.74                     | 0.70              |
| 31:l:36:ALA:N     | 31:l:37:PRO:HD3   | 2.07                     | 0.70              |
| 46:X:14:LEU:O     | 46:X:18:VAL:HG23  | 1.91                     | 0.70              |
| 51:1:1752:C:H6    | 51:1:1752:C:H5'   | 1.56                     | 0.70              |
| 30:H:14:VAL:HG11  | 30:H:180:ASP:OD1  | 1.92                     | 0.69              |
| 40:R:15:VAL:HG23  | 40:R:16:ILE:CD1   | 2.20                     | 0.69              |
| 50:3:225:C:C3'    | 50:3:226:G:H5''   | 2.22                     | 0.69              |
| 1:b:124:LYS:HB3   | 1:b:127:ASN:ND2   | 2.07                     | 0.69              |
| 30:H:111:ASP:HB3  | 30:H:114:LEU:HB2  | 1.74                     | 0.69              |
| 41:S:60:ARG:HH11  | 50:3:981:U:H1'    | 1.57                     | 0.69              |
| 39:Q:2:THR:HB     | 39:Q:5:GLN:HG3    | 1.74                     | 0.69              |
| 42:T:40:GLY:O     | 42:T:44:GLU:HG2   | 1.91                     | 0.69              |
| 7:j:30:THR:HG21   | 51:1:1005:C:O2'   | 1.92                     | 0.69              |
| 50:3:1280:A:O2'   | 50:3:1281:C:H5'   | 1.91                     | 0.69              |
| 2:c:149:ASN:O     | 2:c:152:PRO:HD2   | 1.92                     | 0.69              |
| 29:G:186:VAL:HG13 | 29:G:190:SER:HB2  | 1.74                     | 0.69              |
| 55:8:4:ILE:N      | 55:8:4:ILE:HD12   | 2.07                     | 0.69              |
| 37:O:44:THR:HG23  | 37:O:69:THR:O     | 1.92                     | 0.69              |
| 49:a:30:LEU:HG    | 49:a:178:VAL:HG13 | 1.74                     | 0.69              |
| 22:y:41:HIS:CD2   | 51:1:96:C:H4'     | 2.28                     | 0.69              |
| 9:l:93:ASN:OD1    | 9:l:94:THR:HG23   | 1.92                     | 0.69              |
| 13:p:26:GLU:HB3   | 13:p:84:SER:HB3   | 1.75                     | 0.69              |
| 55:8:93:GLU:HA    | 55:8:96:PHE:HB3   | 1.72                     | 0.69              |
| 16:s:90:LYS:HB2   | 16:s:92:ARG:HH12  | 1.58                     | 0.69              |
| 18:u:81:ARG:HH12  | 51:1:300:A:H3'    | 1.57                     | 0.69              |
| 36:N:57:VAL:HG23  | 36:N:58:GLU:H     | 1.57                     | 0.69              |
| 37:O:43:PRO:HB3   | 50:3:1150:A:H4'   | 1.73                     | 0.69              |
| 48:Z:5:VAL:HG12   | 48:Z:19:LYS:NZ    | 2.07                     | 0.69              |
| 51:1:446:G:H4'    | 51:1:449:A:N3     | 2.08                     | 0.69              |
| 51:1:1664:A:H61   | 51:1:1996:C:H42   | 1.41                     | 0.69              |
| 29:G:156:LEU:HD23 | 29:G:157:PRO:O    | 1.93                     | 0.69              |
| 49:a:16:ASP:HB2   | 49:a:19:LYS:HG2   | 1.73                     | 0.69              |
| 50:3:21:G:H21     | 50:3:914:A:H62    | 1.39                     | 0.69              |
| 35:M:80:PRO:HG2   | 50:3:878:A:H5'    | 1.76                     | 0.68              |
| 4:e:114:ARG:NH1   | 4:e:175:PRO:HD2   | 2.08                     | 0.68              |
| 7:j:26:GLY:HA3    | 51:1:1140:C:H5'   | 1.75                     | 0.68              |
| 29:G:213:LEU:HA   | 29:G:216:VAL:HG22 | 1.73                     | 0.68              |
| 50:3:113:G:H1'    | 50:3:354:G:H5''   | 1.74                     | 0.68              |
| 55:8:144:TRP:CD1  | 55:8:201:LEU:HD22 | 2.29                     | 0.68              |
| 20:w:16:ARG:HD3   | 51:1:2356:U:H4'   | 1.75                     | 0.68              |
| 22:y:17:GLU:HB2   | 22:y:53:VAL:HG11  | 1.76                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:f:102:ILE:HD12  | 5:f:102:ILE:N     | 2.09                     | 0.68              |
| 7:j:101:ILE:H     | 7:j:101:ILE:HD12  | 1.58                     | 0.68              |
| 38:P:24:ALA:HA    | 38:P:29:THR:HA    | 1.76                     | 0.68              |
| 51:1:1422:G:N2    | 51:1:1498:C:H1'   | 2.07                     | 0.68              |
| 10:m:11:LYS:HD2   | 10:m:86:LYS:HD3   | 1.74                     | 0.68              |
| 15:r:15:SER:H     | 15:r:18:GLN:HE21  | 1.39                     | 0.68              |
| 38:P:80:ASN:HA    | 38:P:105:ARG:HB3  | 1.76                     | 0.68              |
| 50:3:216:U:H4'    | 50:3:464:U:H4'    | 1.74                     | 0.68              |
| 51:1:1073:A:N6    | 55:8:54:GLN:HG3   | 2.09                     | 0.68              |
| 51:1:1847:A:H2'   | 51:1:1848:A:H8    | 1.59                     | 0.68              |
| 55:8:354:ASP:O    | 55:8:358:GLU:HG2  | 1.94                     | 0.68              |
| 4:e:73:VAL:HG22   | 4:e:75:GLY:H      | 1.58                     | 0.68              |
| 12:o:51:ALA:HB3   | 12:o:78:VAL:HG22  | 1.76                     | 0.68              |
| 13:p:4:ILE:HD12   | 13:p:4:ILE:N      | 2.08                     | 0.68              |
| 32:J:107:GLY:HA2  | 50:3:8:A:H1'      | 1.75                     | 0.68              |
| 50:3:955:U:H3     | 50:3:1225:A:H61   | 1.39                     | 0.68              |
| 51:1:1874:C:H2'   | 51:1:1875:G:O4'   | 1.94                     | 0.68              |
| 4:e:147:ARG:HB3   | 4:e:149:ARG:NE    | 2.08                     | 0.68              |
| 50:3:730:G:H2'    | 50:3:731:G:H5'    | 1.75                     | 0.68              |
| 3:d:68:ALA:HA     | 51:1:1255:U:C5    | 2.29                     | 0.68              |
| 29:G:15:PHE:HA    | 29:G:39:ILE:HA    | 1.76                     | 0.68              |
| 31:I:10:LEU:HD23  | 31:I:10:LEU:H     | 1.58                     | 0.68              |
| 41:S:74:ARG:HH21  | 50:3:1359:C:H3'   | 1.58                     | 0.68              |
| 42:T:42:PHE:CD2   | 42:T:55:LEU:HD22  | 2.28                     | 0.68              |
| 29:G:32:GLY:HA3   | 29:G:39:ILE:HD13  | 1.76                     | 0.68              |
| 29:G:116:LEU:HD12 | 29:G:143:LEU:HD12 | 1.76                     | 0.68              |
| 45:W:33:THR:HG23  | 45:W:35:SER:H     | 1.59                     | 0.68              |
| 50:3:494:G:H2'    | 50:3:496:A:H1'    | 1.75                     | 0.68              |
| 5:f:154:GLU:HB3   | 5:f:159:LYS:H     | 1.59                     | 0.67              |
| 9:l:61:LEU:O      | 27:E:12:ARG:HD3   | 1.94                     | 0.67              |
| 33:K:10:VAL:HB    | 33:K:58:HIS:HB3   | 1.76                     | 0.67              |
| 35:M:10:LEU:HD22  | 35:M:74:ILE:CD1   | 2.24                     | 0.67              |
| 52:2:3:C:C2'      | 52:2:4:C:H5''     | 2.24                     | 0.67              |
| 55:8:80:VAL:HG22  | 55:8:84:LEU:HD23  | 1.76                     | 0.67              |
| 9:l:30:THR:HG23   | 51:1:810:U:C4     | 2.29                     | 0.67              |
| 15:r:34:GLU:OE2   | 15:r:58:VAL:HG12  | 1.94                     | 0.67              |
| 51:1:2143:C:H2'   | 51:1:2144:G:H5'   | 1.76                     | 0.67              |
| 10:m:45:GLN:HE21  | 51:1:2485:G:C5'   | 2.07                     | 0.67              |
| 11:n:2:ARG:HA     | 11:n:5:LYS:HD3    | 1.73                     | 0.67              |
| 33:K:11:HIS:CE1   | 33:K:53:LYS:HE3   | 2.28                     | 0.67              |
| 36:N:5:TYR:HD2    | 36:N:20:ILE:HG23  | 1.60                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:U:19:VAL:HG13  | 43:U:36:VAL:HG13  | 1.77                     | 0.67              |
| 49:a:42:VAL:HG13  | 49:a:215:SER:O    | 1.95                     | 0.67              |
| 10:m:41:LEU:HD23  | 10:m:96:ILE:HG13  | 1.77                     | 0.67              |
| 15:r:41:ILE:HD11  | 15:r:57:GLY:HA3   | 1.77                     | 0.67              |
| 38:P:93:GLU:O     | 38:P:97:ARG:HG3   | 1.94                     | 0.67              |
| 50:3:1237:C:OP1   | 50:3:1238:A:H1'   | 1.93                     | 0.67              |
| 51:1:1717:A:H62   | 51:1:1743:G:H21   | 1.43                     | 0.67              |
| 12:o:71:ALA:HB1   | 12:o:106:LEU:HB2  | 1.76                     | 0.67              |
| 32:J:105:ILE:HD11 | 32:J:123:LEU:HD22 | 1.76                     | 0.67              |
| 32:J:108:GLY:H    | 50:3:9:G:C5'      | 2.08                     | 0.67              |
| 34:L:47:GLU:O     | 34:L:51:GLN:HG2   | 1.94                     | 0.67              |
| 51:1:2105:U:C2'   | 51:1:2106:U:H5'   | 2.24                     | 0.67              |
| 51:1:2143:C:C2'   | 51:1:2144:G:H5'   | 2.24                     | 0.67              |
| 13:p:109:ILE:N    | 13:p:109:ILE:HD12 | 2.09                     | 0.67              |
| 41:S:73:LEU:HD13  | 41:S:76:PHE:HD2   | 1.59                     | 0.67              |
| 49:a:24:ASN:HD22  | 49:a:186:LYS:HE3  | 1.59                     | 0.67              |
| 1:b:204:LEU:HD22  | 1:b:213:ARG:HE    | 1.59                     | 0.67              |
| 12:o:34:HIS:C     | 12:o:35:ILE:HD12  | 2.20                     | 0.67              |
| 17:t:61:LEU:HB3   | 51:1:1341:G:H4'   | 1.76                     | 0.67              |
| 4:e:124:ARG:N     | 4:e:124:ARG:HD2   | 2.09                     | 0.67              |
| 51:1:2508:G:H1    | 51:1:2580:U:H5    | 1.43                     | 0.67              |
| 24:B:13:GLY:HA3   | 51:1:16:C:H5''    | 1.76                     | 0.67              |
| 32:J:104:ILE:HD12 | 32:J:122:VAL:O    | 1.94                     | 0.67              |
| 34:L:28:ILE:CG2   | 34:L:104:VAL:HG21 | 2.25                     | 0.67              |
| 39:Q:23:LEU:CD2   | 39:Q:29:LYS:HD3   | 2.24                     | 0.67              |
| 41:S:5:MET:HE3    | 41:S:62:ARG:HH22  | 1.58                     | 0.67              |
| 43:U:14:ARG:HH12  | 50:3:618:C:H1'    | 1.59                     | 0.67              |
| 1:b:28:PRO:HG2    | 1:b:33:LEU:HD21   | 1.77                     | 0.67              |
| 4:e:107:VAL:N     | 4:e:108:PRO:HD2   | 2.10                     | 0.67              |
| 6:g:9:VAL:HG23    | 6:g:13:GLY:HA3    | 1.75                     | 0.67              |
| 6:g:47:PHE:HA     | 6:g:51:ARG:HB2    | 1.76                     | 0.67              |
| 13:p:47:ILE:N     | 13:p:47:ILE:HD12  | 2.09                     | 0.67              |
| 50:3:346:G:C2'    | 50:3:347:G:H5'    | 2.24                     | 0.67              |
| 51:1:63:A:H2'     | 51:1:64:A:C8      | 2.30                     | 0.67              |
| 51:1:1454:C:H2'   | 51:1:1455:G:H5'   | 1.77                     | 0.67              |
| 6:g:40:THR:CG2    | 6:g:43:ASN:HD22   | 2.08                     | 0.66              |
| 30:H:120:THR:HG23 | 30:H:188:ALA:HA   | 1.75                     | 0.66              |
| 51:1:85:G:C3'     | 51:1:86:G:H5''    | 2.25                     | 0.66              |
| 51:1:1079:C:H2'   | 51:1:1080:A:C8    | 2.31                     | 0.66              |
| 51:1:1915:U:O4'   | 55:8:311:GLU:HG3  | 1.95                     | 0.66              |
| 5:f:71:LEU:O      | 5:f:75:VAL:HG23   | 1.95                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:G:116:LEU:HB3  | 29:G:140:LEU:HD21 | 1.75                     | 0.66              |
| 51:1:161:A:H3'    | 51:1:162:U:H5''   | 1.77                     | 0.66              |
| 51:1:1450:G:H21   | 51:1:1452:G:H1    | 1.40                     | 0.66              |
| 1:b:86:ARG:HG3    | 1:b:86:ARG:HH11   | 1.59                     | 0.66              |
| 15:r:27:ILE:HG23  | 15:r:28:ALA:N     | 2.08                     | 0.66              |
| 41:S:26:LEU:HA    | 41:S:30:ILE:HD13  | 1.77                     | 0.66              |
| 51:1:884:U:H3     | 51:1:892:A:H61    | 1.43                     | 0.66              |
| 18:u:16:LYS:HG2   | 51:1:329:G:H1     | 1.60                     | 0.66              |
| 22:y:47:ARG:O     | 22:y:50:VAL:HG12  | 1.93                     | 0.66              |
| 40:R:89:ARG:HH22  | 50:3:1321:U:H4'   | 1.61                     | 0.66              |
| 47:Y:2:ASN:O      | 47:Y:7:LYS:HE3    | 1.96                     | 0.66              |
| 34:L:4:ARG:HH22   | 50:3:1345:U:H2'   | 1.61                     | 0.66              |
| 36:N:53:LEU:HD22  | 36:N:97:LEU:HD23  | 1.76                     | 0.66              |
| 44:V:16:MET:HB3   | 44:V:19:SER:HB2   | 1.77                     | 0.66              |
| 49:a:162:ARG:HH11 | 49:a:164:ARG:HE   | 1.44                     | 0.66              |
| 4:e:123:GLY:C     | 4:e:124:ARG:HD2   | 2.20                     | 0.66              |
| 6:g:108:VAL:HG12  | 6:g:110:VAL:HG23  | 1.78                     | 0.66              |
| 12:o:94:ARG:NH2   | 51:1:2293:G:H5''  | 2.11                     | 0.66              |
| 29:G:101:THR:CG2  | 50:3:1074:G:H4'   | 2.26                     | 0.66              |
| 31:I:131:ILE:HD12 | 31:I:131:ILE:N    | 2.10                     | 0.66              |
| 37:O:41:PRO:HG3   | 50:3:1150:A:N3    | 2.11                     | 0.66              |
| 51:1:1179:G:C2'   | 51:1:1180:U:H4'   | 2.24                     | 0.66              |
| 35:M:54:THR:HG23  | 35:M:55:LYS:HG3   | 1.78                     | 0.66              |
| 39:Q:117:GLY:HA2  | 50:3:35:G:O2'     | 1.96                     | 0.66              |
| 50:3:1139:G:H5''  | 50:3:1140:C:H5    | 1.61                     | 0.66              |
| 51:1:85:G:H2'     | 51:1:86:G:H5''    | 1.78                     | 0.66              |
| 51:1:783:A:H2'    | 51:1:784:G:C4'    | 2.23                     | 0.66              |
| 51:1:845:A:H3'    | 51:1:846:U:H5''   | 1.78                     | 0.66              |
| 51:1:2134:A:N6    | 51:1:2157:G:H4'   | 2.10                     | 0.66              |
| 1:b:19:VAL:HG22   | 1:b:20:ASN:H      | 1.61                     | 0.66              |
| 7:j:47:HIS:CE1    | 7:j:48:VAL:HG13   | 2.30                     | 0.66              |
| 8:k:102:PRO:HD3   | 13:p:65:ASN:HD22  | 1.60                     | 0.66              |
| 32:J:44:ARG:HB3   | 32:J:70:MET:HG2   | 1.77                     | 0.66              |
| 38:P:114:PRO:HB3  | 50:3:676:A:H5''   | 1.76                     | 0.66              |
| 50:3:1071:C:H2'   | 50:3:1072:G:H8    | 1.61                     | 0.66              |
| 55:8:128:CYS:HB3  | 55:8:189:TYR:HB2  | 1.78                     | 0.66              |
| 55:8:153:LEU:HD12 | 55:8:154:ARG:N    | 2.11                     | 0.66              |
| 7:j:24:THR:HG23   | 7:j:27:ARG:HB2    | 1.77                     | 0.66              |
| 18:u:1:ALA:HB2    | 51:1:83:A:OP1     | 1.95                     | 0.66              |
| 4:e:142:TYR:HA    | 4:e:145:VAL:HG12  | 1.77                     | 0.66              |
| 29:G:116:LEU:HD21 | 29:G:139:GLU:OE2  | 1.95                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 35:M:101:ALA:HB3 | 35:M:112:ASP:HB3 | 1.78                     | 0.66              |
| 23:z:15:ARG:HG3  | 23:z:53:MET:HE1  | 1.77                     | 0.65              |
| 39:Q:72:ASN:ND2  | 39:Q:98:ARG:NE   | 2.44                     | 0.65              |
| 44:V:11:VAL:HG13 | 44:V:20:ILE:HD11 | 1.77                     | 0.65              |
| 50:3:1497:G:O2'  | 50:3:1498:U:H5'  | 1.96                     | 0.65              |
| 51:1:729:G:O2'   | 51:1:763:G:H4'   | 1.96                     | 0.65              |
| 6:g:32:PRO:HG2   | 6:g:33:GLN:OE1   | 1.96                     | 0.65              |
| 13:p:83:ILE:HD12 | 13:p:83:ILE:N    | 2.11                     | 0.65              |
| 13:p:90:ALA:HB2  | 13:p:112:ARG:HA  | 1.77                     | 0.65              |
| 16:s:3:THR:HG21  | 16:s:58:ALA:HA   | 1.77                     | 0.65              |
| 18:u:87:GLU:HG3  | 18:u:88:ASP:OD1  | 1.96                     | 0.65              |
| 29:G:94:ARG:NH2  | 50:3:1102:A:H4'  | 2.10                     | 0.65              |
| 31:I:85:THR:HA   | 31:I:88:ASN:HD22 | 1.60                     | 0.65              |
| 41:S:47:LEU:HD23 | 41:S:47:LEU:O    | 1.96                     | 0.65              |
| 51:1:1558:C:H5'' | 51:1:1559:U:H3'  | 1.79                     | 0.65              |
| 3:d:181:ILE:HG23 | 9:l:2:ARG:HG3    | 1.77                     | 0.65              |
| 12:o:33:ARG:HG3  | 52:2:52:A:H62    | 1.62                     | 0.65              |
| 22:y:19:LEU:HB3  | 22:y:23:ARG:NH2  | 2.11                     | 0.65              |
| 51:1:479:A:H4'   | 51:1:480:A:H5'   | 1.76                     | 0.65              |
| 55:8:11:ILE:CD1  | 55:8:80:VAL:HG11 | 2.26                     | 0.65              |
| 55:8:11:ILE:HD12 | 55:8:80:VAL:HG11 | 1.77                     | 0.65              |
| 55:8:164:GLU:HB3 | 55:8:182:LYS:HB3 | 1.76                     | 0.65              |
| 10:m:78:LEU:O    | 55:8:282:LYS:NZ  | 2.30                     | 0.65              |
| 19:v:80:HIS:CG   | 19:v:83:LYS:HB2  | 2.32                     | 0.65              |
| 31:I:30:LYS:HE2  | 50:3:411:A:O2'   | 1.95                     | 0.65              |
| 50:3:1412:C:H2'  | 50:3:1413:A:C8   | 2.32                     | 0.65              |
| 6:g:26:ALA:HA    | 6:g:30:LEU:HD12  | 1.79                     | 0.65              |
| 28:F:4:ARG:HB3   | 51:1:2466:C:OP1  | 1.95                     | 0.65              |
| 36:N:83:THR:HG23 | 36:N:97:LEU:HD13 | 1.78                     | 0.65              |
| 40:R:22:TYR:CD2  | 40:R:65:GLU:HG3  | 2.31                     | 0.65              |
| 50:3:1130:A:H61  | 50:3:1144:G:H1'  | 1.61                     | 0.65              |
| 51:1:2542:A:H4'  | 51:1:2543:G:H5'  | 1.78                     | 0.65              |
| 55:8:11:ILE:HD12 | 55:8:80:VAL:HG21 | 1.79                     | 0.65              |
| 4:e:114:ARG:CZ   | 4:e:175:PRO:HD2  | 2.27                     | 0.65              |
| 16:s:6:LYS:HG3   | 51:1:494:G:H4'   | 1.79                     | 0.65              |
| 51:1:49:A:H5'    | 51:1:51:G:O4'    | 1.96                     | 0.65              |
| 4:e:90:LEU:HD22  | 4:e:94:ARG:HD3   | 1.79                     | 0.65              |
| 11:n:22:ARG:HH12 | 51:1:2709:G:H5'  | 1.62                     | 0.65              |
| 38:P:55:ARG:O    | 38:P:58:THR:HG22 | 1.96                     | 0.65              |
| 9:l:30:THR:HG23  | 51:1:810:U:N3    | 2.11                     | 0.65              |
| 14:q:91:ARG:HD3  | 51:1:997:G:OP1   | 1.97                     | 0.65              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 29:G:39:ILE:H     | 29:G:39:ILE:HD12 | 1.62                     | 0.65              |
| 31:I:64:TYR:HA    | 31:I:110:ARG:HD2 | 1.78                     | 0.65              |
| 44:V:37:ILE:H     | 44:V:37:ILE:HD12 | 1.62                     | 0.65              |
| 51:1:277:G:H5'    | 51:1:278:A:H5'   | 1.78                     | 0.65              |
| 51:1:503:A:H4'    | 51:1:505:A:H5''  | 1.77                     | 0.65              |
| 4:e:132:ARG:HB2   | 4:e:133:GLU:OE2  | 1.96                     | 0.65              |
| 21:x:76:LYS:HE3   | 51:1:153:U:OP1   | 1.97                     | 0.65              |
| 39:Q:72:ASN:HD21  | 39:Q:98:ARG:NE   | 1.95                     | 0.65              |
| 51:1:1079:C:H2'   | 51:1:1080:A:H8   | 1.62                     | 0.65              |
| 20:w:68:LYS:HB2   | 20:w:75:PHE:CD2  | 2.32                     | 0.65              |
| 50:3:1532:U:H3'   | 50:3:1533:C:H5'' | 1.78                     | 0.65              |
| 4:e:49:LEU:HD11   | 4:e:85:GLY:HA2   | 1.79                     | 0.64              |
| 5:f:24:THR:HG22   | 5:f:33:THR:HG23  | 1.78                     | 0.64              |
| 6:g:77:THR:HG22   | 6:g:143:ILE:HB   | 1.78                     | 0.64              |
| 7:j:45:THR:HB     | 7:j:48:VAL:CG2   | 2.26                     | 0.64              |
| 10:m:18:ARG:HD2   | 52:2:90:C:H5'    | 1.79                     | 0.64              |
| 31:I:80:ARG:HG2   | 31:I:80:ARG:HH11 | 1.62                     | 0.64              |
| 38:P:66:ALA:HB3   | 38:P:98:ALA:CB   | 2.26                     | 0.64              |
| 41:S:8:ARG:HA     | 41:S:11:LYS:HD2  | 1.77                     | 0.64              |
| 42:T:17:ASP:OD2   | 42:T:19:ASN:HB2  | 1.98                     | 0.64              |
| 49:a:23:ILE:HA    | 49:a:224:VAL:HB  | 1.79                     | 0.64              |
| 55:8:33:ARG:HH11  | 55:8:36:GLU:HB3  | 1.62                     | 0.64              |
| 8:k:42:THR:HG22   | 8:k:57:VAL:HG22  | 1.77                     | 0.64              |
| 10:m:63:ILE:HG12  | 10:m:105:MET:SD  | 2.37                     | 0.64              |
| 16:s:90:LYS:HB2   | 16:s:92:ARG:NH1  | 2.12                     | 0.64              |
| 21:x:65:THR:O     | 21:x:69:GLU:HG3  | 1.97                     | 0.64              |
| 31:I:58:GLN:HG3   | 50:3:544:G:OP1   | 1.96                     | 0.64              |
| 35:M:77:VAL:HG12  | 35:M:84:ILE:HD12 | 1.78                     | 0.64              |
| 37:O:52:LEU:CD1   | 41:S:80:ARG:HE   | 2.11                     | 0.64              |
| 38:P:83:VAL:HB    | 38:P:109:ILE:HA  | 1.78                     | 0.64              |
| 51:1:1697:G:H4'   | 51:1:1978:A:H5'' | 1.80                     | 0.64              |
| 10:m:76:LYS:HG2   | 10:m:80:VAL:CG1  | 2.28                     | 0.64              |
| 21:x:56:ARG:HB3   | 51:1:372:G:N7    | 2.12                     | 0.64              |
| 40:R:106:ARG:NH1  | 40:R:106:ARG:HB3 | 2.12                     | 0.64              |
| 50:3:1345:U:H4'   | 50:3:1346:A:H8   | 1.62                     | 0.64              |
| 16:s:77:ASP:OD1   | 16:s:102:HIS:HB2 | 1.98                     | 0.64              |
| 47:Y:77:ASN:O     | 47:Y:81:GLN:HG2  | 1.97                     | 0.64              |
| 55:8:161:PHE:CD1  | 55:8:185:GLY:HA3 | 2.33                     | 0.64              |
| 9:l:62:PRO:HB2    | 27:E:29:ARG:HH11 | 1.61                     | 0.64              |
| 13:p:47:ILE:HD12  | 13:p:47:ILE:H    | 1.63                     | 0.64              |
| 32:J:152:VAL:HG21 | 35:M:98:LEU:HD11 | 1.80                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:M:3:GLN:HB2    | 50:3:587:G:H4'    | 1.78                     | 0.64              |
| 37:O:52:LEU:HD11  | 41:S:80:ARG:NH2   | 2.12                     | 0.64              |
| 49:a:161:VAL:HG11 | 49:a:174:THR:HG22 | 1.78                     | 0.64              |
| 50:3:1170:A:H2'   | 50:3:1171:A:H5'   | 1.80                     | 0.64              |
| 51:1:2130:U:H5'   | 51:1:2159:G:H22   | 1.63                     | 0.64              |
| 32:J:93:VAL:HG21  | 32:J:110:MET:SD   | 2.38                     | 0.64              |
| 38:P:121:ARG:HH12 | 38:P:124:LYS:HG2  | 1.61                     | 0.64              |
| 55:8:238:ASP:HA   | 55:8:266:ILE:HD11 | 1.79                     | 0.64              |
| 4:e:79:ARG:HG3    | 4:e:80:GLN:H      | 1.63                     | 0.64              |
| 46:X:39:ILE:HG21  | 46:X:65:MET:HB3   | 1.79                     | 0.64              |
| 50:3:206:C:H2'    | 50:3:207:C:O4'    | 1.98                     | 0.64              |
| 55:8:338:THR:HG21 | 55:8:360:SER:HA   | 1.78                     | 0.64              |
| 28:F:19:ARG:HB2   | 28:F:24:ARG:HD2   | 1.80                     | 0.64              |
| 31:I:117:VAL:HG11 | 31:I:132:ALA:HB2  | 1.80                     | 0.64              |
| 42:T:63:ARG:HH22  | 42:T:87:ARG:NH1   | 1.95                     | 0.64              |
| 50:3:952:U:H4'    | 50:3:964:A:H61    | 1.63                     | 0.64              |
| 55:8:176:ILE:HD12 | 55:8:179:VAL:HG11 | 1.79                     | 0.64              |
| 3:d:117:ARG:NH1   | 9:l:2:ARG:HG2     | 2.13                     | 0.64              |
| 3:d:149:ILE:HG23  | 3:d:188:MET:HA    | 1.80                     | 0.64              |
| 12:o:33:ARG:HG3   | 52:2:52:A:N6      | 2.12                     | 0.64              |
| 30:H:166:TRP:HZ3  | 30:H:168:ARG:HB2  | 1.63                     | 0.64              |
| 32:J:40:ASP:OD2   | 32:J:42:ASN:HB2   | 1.98                     | 0.64              |
| 50:3:1005:A:H2'   | 50:3:1006:G:O4'   | 1.97                     | 0.64              |
| 50:3:1493:A:H1'   | 55:8:136:SER:HA   | 1.78                     | 0.64              |
| 51:1:1470:A:H62   | 51:1:1521:G:H21   | 1.45                     | 0.64              |
| 17:t:10:VAL:HG11  | 17:t:42:GLU:OE1   | 1.98                     | 0.63              |
| 31:I:8:LEU:HD12   | 50:3:429:U:H3'    | 1.80                     | 0.63              |
| 41:S:58:ARG:HH21  | 50:3:980:C:H4'    | 1.63                     | 0.63              |
| 51:1:1270:C:H5''  | 51:1:1271:G:C5'   | 2.24                     | 0.63              |
| 4:e:24:VAL:HG13   | 4:e:25:MET:HE2    | 1.80                     | 0.63              |
| 17:t:56:GLU:OE2   | 17:t:88:LYS:HG2   | 1.98                     | 0.63              |
| 30:H:127:VAL:HG22 | 30:H:128:MET:N    | 2.13                     | 0.63              |
| 34:L:24:LYS:HE2   | 50:3:1375:A:H5''  | 1.79                     | 0.63              |
| 41:S:40:ARG:NH2   | 46:X:6:LYS:HB3    | 2.13                     | 0.63              |
| 50:3:29:U:O2'     | 50:3:30:U:H5'     | 1.98                     | 0.63              |
| 50:3:811:C:H4'    | 50:3:901:A:H61    | 1.62                     | 0.63              |
| 51:1:799:G:H5''   | 51:1:800:A:H2'    | 1.80                     | 0.63              |
| 55:8:242:ASP:HB2  | 55:8:262:ARG:HB3  | 1.80                     | 0.63              |
| 5:f:90:GLY:HA3    | 5:f:93:TYR:CD2    | 2.33                     | 0.63              |
| 8:k:5:GLN:HG3     | 51:1:1669:A:O4'   | 1.98                     | 0.63              |
| 31:I:33:ILE:HD12  | 31:I:33:ILE:N     | 2.14                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 38:P:27:ASN:HA   | 38:P:57:SER:OG    | 1.99                     | 0.63              |
| 41:S:62:ARG:HH21 | 50:3:981:U:H5''   | 1.61                     | 0.63              |
| 44:V:15:LYS:HE3  | 50:3:275:G:O5'    | 1.97                     | 0.63              |
| 50:3:1412:C:H2'  | 50:3:1413:A:H8    | 1.63                     | 0.63              |
| 51:1:745:G:O2'   | 51:1:748:G:H1'    | 1.99                     | 0.63              |
| 51:1:2452:C:H42  | 51:1:2504:U:H3    | 1.44                     | 0.63              |
| 53:5:15:G:N2     | 53:5:48:C:H42     | 1.88                     | 0.63              |
| 55:8:266:ILE:CG1 | 55:8:267:PRO:HD3  | 2.28                     | 0.63              |
| 37:O:76:ILE:N    | 37:O:76:ILE:HD12  | 2.13                     | 0.63              |
| 45:W:53:GLN:HA   | 45:W:56:ARG:HH12  | 1.63                     | 0.63              |
| 5:f:137:LYS:CD   | 51:1:2746:U:H5''  | 2.29                     | 0.63              |
| 9:l:53:GLY:HA3   | 51:1:826:U:O2'    | 1.98                     | 0.63              |
| 19:v:72:VAL:HA   | 19:v:94:ALA:H     | 1.63                     | 0.63              |
| 29:G:135:MET:O   | 29:G:139:GLU:HG2  | 1.98                     | 0.63              |
| 46:X:2:ARG:HG2   | 50:3:1312:G:C8    | 2.33                     | 0.63              |
| 8:k:76:VAL:H     | 13:p:72:VAL:CG2   | 2.11                     | 0.63              |
| 29:G:207:ARG:O   | 29:G:211:LEU:HD23 | 1.99                     | 0.63              |
| 50:3:868:C:H2'   | 50:3:869:G:O4'    | 1.99                     | 0.63              |
| 55:8:144:TRP:CE2 | 55:8:201:LEU:HB2  | 2.34                     | 0.63              |
| 3:d:41:GLN:HG2   | 3:d:43:THR:HG23   | 1.81                     | 0.63              |
| 15:r:93:PHE:HE2  | 15:r:95:ASP:OD2   | 1.81                     | 0.63              |
| 31:I:28:ASP:OD1  | 31:I:31:CYS:HB3   | 1.98                     | 0.63              |
| 51:1:2051:A:H2'  | 51:1:2578:G:OP1   | 1.99                     | 0.63              |
| 1:b:1:ALA:N      | 1:b:19:VAL:O      | 2.32                     | 0.63              |
| 7:j:101:ILE:HD12 | 7:j:101:ILE:N     | 2.14                     | 0.63              |
| 17:t:10:VAL:HG11 | 17:t:42:GLU:CD    | 2.23                     | 0.63              |
| 35:M:9:MET:O     | 35:M:13:ILE:HG13  | 1.99                     | 0.63              |
| 2:c:149:ASN:HD21 | 51:1:2572:A:H5''  | 1.64                     | 0.62              |
| 5:f:171:LYS:HD3  | 51:1:2530:A:H62   | 1.63                     | 0.62              |
| 51:1:366:C:H3'   | 51:1:367:G:H5''   | 1.81                     | 0.62              |
| 51:1:774:G:C2'   | 51:1:775:G:H5''   | 2.28                     | 0.62              |
| 6:g:147:VAL:HG22 | 6:g:148:ALA:H     | 1.64                     | 0.62              |
| 8:k:70:ARG:HG2   | 8:k:76:VAL:HG12   | 1.79                     | 0.62              |
| 10:m:63:ILE:HG12 | 10:m:105:MET:HE1  | 1.81                     | 0.62              |
| 16:s:25:ARG:HE   | 16:s:74:ILE:HG23  | 1.64                     | 0.62              |
| 29:G:4:SER:O     | 29:G:8:MET:HG2    | 1.98                     | 0.62              |
| 39:Q:53:ARG:HA   | 39:Q:63:THR:HA    | 1.81                     | 0.62              |
| 40:R:9:PRO:HB2   | 40:R:44:ILE:HD12  | 1.81                     | 0.62              |
| 30:H:42:LEU:HD23 | 30:H:54:ILE:HD13  | 1.80                     | 0.62              |
| 38:P:85:VAL:HG21 | 38:P:92:ARG:HG3   | 1.81                     | 0.62              |
| 43:U:53:ASP:OD2  | 43:U:56:ARG:HG2   | 1.99                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 51:1:288:U:H2'   | 51:1:289:G:C8     | 2.34                     | 0.62              |
| 51:1:2800:A:C3'  | 51:1:2801:G:H5'   | 2.22                     | 0.62              |
| 1:b:200:MET:HG3  | 1:b:201:LEU:HD12  | 1.82                     | 0.62              |
| 3:d:48:THR:HG23  | 3:d:50:ALA:H      | 1.64                     | 0.62              |
| 9:l:17:LYS:HD3   | 51:1:663:G:H5''   | 1.80                     | 0.62              |
| 45:W:59:LYS:HD3  | 50:3:734:G:O2'    | 1.99                     | 0.62              |
| 48:Z:39:LYS:O    | 48:Z:43:GLU:N     | 2.30                     | 0.62              |
| 2:c:61:THR:HB    | 2:c:63:PRO:HD2    | 1.82                     | 0.62              |
| 14:q:106:THR:O   | 14:q:110:GLU:HG3  | 1.99                     | 0.62              |
| 28:F:27:CYS:SG   | 28:F:30:GLU:HB2   | 2.39                     | 0.62              |
| 32:J:101:GLY:H   | 32:J:121:ASN:HB2  | 1.65                     | 0.62              |
| 32:J:133:ILE:O   | 32:J:136:VAL:HG22 | 1.99                     | 0.62              |
| 37:O:56:HIS:CE1  | 50:3:963:G:H21    | 2.17                     | 0.62              |
| 49:a:169:GLY:C   | 49:a:170:ILE:HD12 | 2.24                     | 0.62              |
| 51:1:974:G:H1'   | 51:1:975:A:C8     | 2.34                     | 0.62              |
| 51:1:1285:A:H2'  | 51:1:1286:A:H5'   | 1.82                     | 0.62              |
| 51:1:2179:C:H2'  | 51:1:2180:U:H5    | 1.65                     | 0.62              |
| 51:1:2590:A:N1   | 51:1:2604:U:H5    | 1.96                     | 0.62              |
| 53:5:47:U:H4'    | 53:5:48:C:H5''    | 1.80                     | 0.62              |
| 4:e:159:ALA:HB1  | 4:e:164:GLU:HB2   | 1.82                     | 0.62              |
| 12:o:68:LYS:HA   | 12:o:102:ARG:HG2  | 1.81                     | 0.62              |
| 30:H:112:ALA:CB  | 30:H:184:ASN:HD22 | 2.10                     | 0.62              |
| 31:I:10:LEU:HD21 | 31:I:20:LEU:HD13  | 1.80                     | 0.62              |
| 34:L:107:ALA:HA  | 34:L:122:GLU:HG3  | 1.82                     | 0.62              |
| 51:1:2277:G:C3'  | 51:1:2278:A:H5''  | 2.30                     | 0.62              |
| 51:1:2350:C:H2'  | 51:1:2351:G:O4'   | 1.99                     | 0.62              |
| 51:1:2504:U:C3'  | 51:1:2505:G:H5''  | 2.29                     | 0.62              |
| 1:b:231:HIS:CE1  | 1:b:244:VAL:H     | 2.18                     | 0.62              |
| 13:p:24:THR:CG2  | 13:p:87:ARG:HG3   | 2.30                     | 0.62              |
| 13:p:74:GLN:HB2  | 13:p:77:SER:HB2   | 1.82                     | 0.62              |
| 35:M:125:ILE:H   | 35:M:125:ILE:HD12 | 1.64                     | 0.62              |
| 41:S:25:GLU:HA   | 41:S:28:ALA:HB3   | 1.81                     | 0.62              |
| 47:Y:25:SER:OG   | 50:3:1458:G:H5''  | 1.99                     | 0.62              |
| 55:8:79:ASP:O    | 55:8:83:LEU:HG    | 2.00                     | 0.62              |
| 2:c:148:GLN:O    | 51:1:2052:A:H4'   | 2.00                     | 0.62              |
| 33:K:11:HIS:ND1  | 33:K:53:LYS:HE3   | 2.15                     | 0.62              |
| 37:O:59:LYS:HE2  | 37:O:62:ARG:HH21  | 1.65                     | 0.62              |
| 51:1:899:A:H2'   | 51:1:900:A:C8     | 2.34                     | 0.62              |
| 51:1:2122:U:H2'  | 51:1:2123:G:H5'   | 1.80                     | 0.62              |
| 5:f:104:LEU:HB2  | 5:f:112:VAL:HB    | 1.82                     | 0.62              |
| 17:t:1:MET:HE3   | 17:t:2:ILE:H      | 1.64                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:I:205:LYS:HA   | 50:3:8:A:N7       | 2.14                     | 0.62              |
| 39:Q:74:GLN:H     | 39:Q:76:HIS:CE1   | 2.18                     | 0.62              |
| 42:T:25:GLU:OE1   | 42:T:76:ARG:HD3   | 2.00                     | 0.62              |
| 51:1:1597:A:H5''  | 51:1:1598:A:H5'   | 1.81                     | 0.62              |
| 1:b:204:LEU:HD22  | 1:b:213:ARG:NE    | 2.14                     | 0.62              |
| 34:L:22:LEU:O     | 34:L:26:VAL:HG23  | 2.00                     | 0.62              |
| 34:L:68:VAL:HG21  | 34:L:103:ILE:HD11 | 1.82                     | 0.62              |
| 50:3:1024:G:H2'   | 50:3:1025:U:H5'   | 1.80                     | 0.62              |
| 55:8:166:ILE:HD11 | 55:8:182:LYS:HB2  | 1.81                     | 0.62              |
| 4:e:137:PHE:O     | 4:e:139:GLU:N     | 2.33                     | 0.61              |
| 5:f:34:ARG:HH22   | 51:1:2759:G:H1'   | 1.65                     | 0.61              |
| 15:r:15:SER:H     | 15:r:18:GLN:NE2   | 1.98                     | 0.61              |
| 21:x:2:ARG:HD2    | 51:1:1365:A:OP1   | 2.00                     | 0.61              |
| 55:8:70:LEU:HD21  | 55:8:113:LEU:HD11 | 1.82                     | 0.61              |
| 3:d:137:LYS:O     | 3:d:141:MET:HG2   | 2.00                     | 0.61              |
| 50:3:1125:U:H2'   | 50:3:1126:U:H2'   | 1.82                     | 0.61              |
| 27:E:31:ILE:HG23  | 27:E:31:ILE:O     | 2.00                     | 0.61              |
| 31:I:59:LYS:O     | 31:I:63:ILE:HG13  | 2.00                     | 0.61              |
| 39:Q:52:CYS:HB2   | 39:Q:66:ILE:HD11  | 1.82                     | 0.61              |
| 42:T:55:LEU:HD12  | 42:T:58:MET:SD    | 2.40                     | 0.61              |
| 43:U:33:ILE:N     | 43:U:33:ILE:HD12  | 2.15                     | 0.61              |
| 52:2:66:A:H2'     | 52:2:107:G:O6     | 2.00                     | 0.61              |
| 2:c:22:ILE:N      | 2:c:22:ILE:HD12   | 2.16                     | 0.61              |
| 3:d:70:SER:HG     | 3:d:78:TRP:HZ2    | 1.49                     | 0.61              |
| 12:o:94:ARG:HH22  | 51:1:2293:G:H5''  | 1.65                     | 0.61              |
| 13:p:108:ARG:HD2  | 50:3:1463:U:OP1   | 2.01                     | 0.61              |
| 40:R:100:ARG:HE   | 40:R:103:THR:HG22 | 1.64                     | 0.61              |
| 47:Y:44:ALA:O     | 47:Y:48:LYS:HG2   | 2.00                     | 0.61              |
| 47:Y:69:ASN:HD22  | 50:3:262:A:H4'    | 1.64                     | 0.61              |
| 51:1:2295:C:O2'   | 51:1:2296:U:H5'   | 2.00                     | 0.61              |
| 27:E:18:LYS:CG    | 51:1:651:G:H5'    | 2.26                     | 0.61              |
| 33:K:23:GLU:HA    | 33:K:26:THR:CG2   | 2.30                     | 0.61              |
| 51:1:281:C:H42    | 51:1:359:G:H1     | 1.48                     | 0.61              |
| 51:1:403:U:O3'    | 51:1:404:A:H4'    | 2.00                     | 0.61              |
| 51:1:1186:G:H2'   | 51:1:1187:G:O4'   | 2.01                     | 0.61              |
| 51:1:1554:U:H3'   | 51:1:1555:G:H5'   | 1.83                     | 0.61              |
| 51:1:2563:U:H2'   | 51:1:2564:A:H5''  | 1.82                     | 0.61              |
| 55:8:282:LYS:O    | 55:8:286:GLN:HG3  | 2.00                     | 0.61              |
| 24:B:2:VAL:HG22   | 24:B:3:GLN:N      | 2.15                     | 0.61              |
| 52:2:15:A:H5''    | 52:2:108:A:H4'    | 1.82                     | 0.61              |
| 17:t:74:ILE:N     | 17:t:74:ILE:HD12  | 2.14                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:I:112:GLU:HG3  | 50:3:407:U:O2'    | 2.01                     | 0.61              |
| 32:J:55:VAL:CG2   | 32:J:56:PRO:HD3   | 2.14                     | 0.61              |
| 32:J:108:GLY:H    | 50:3:9:G:H4'      | 1.65                     | 0.61              |
| 40:R:15:VAL:HG11  | 40:R:40:GLU:OE2   | 2.01                     | 0.61              |
| 50:3:946:A:H2'    | 50:3:947:G:C8     | 2.36                     | 0.61              |
| 50:3:1506:U:O2'   | 50:3:1507:A:H5'   | 2.01                     | 0.61              |
| 10:m:109:PRO:HD2  | 10:m:112:LEU:HD23 | 1.83                     | 0.61              |
| 17:t:1:MET:HG3    | 17:t:3:ARG:H      | 1.66                     | 0.61              |
| 25:C:24:LYS:HE2   | 25:C:29:LYS:HB2   | 1.83                     | 0.61              |
| 31:I:72:ARG:HH12  | 31:I:203:TYR:HB3  | 1.64                     | 0.61              |
| 33:K:18:VAL:O     | 33:K:22:ILE:HG13  | 2.01                     | 0.61              |
| 33:K:56:LYS:H     | 33:K:56:LYS:HD2   | 1.64                     | 0.61              |
| 47:Y:2:ASN:ND2    | 47:Y:3:ILE:HG13   | 2.15                     | 0.61              |
| 3:d:118:LEU:HD23  | 3:d:119:ILE:N     | 2.15                     | 0.61              |
| 15:r:38:VAL:HG21  | 15:r:41:ILE:HD11  | 1.83                     | 0.61              |
| 25:C:24:LYS:HG2   | 25:C:25:ASN:N     | 2.15                     | 0.61              |
| 30:H:168:ARG:CZ   | 50:3:1107:C:H4'   | 2.29                     | 0.61              |
| 33:K:3:HIS:CD2    | 33:K:94:HIS:HA    | 2.35                     | 0.61              |
| 40:R:33:LEU:HD12  | 40:R:38:ILE:HB    | 1.81                     | 0.61              |
| 44:V:37:ILE:HD12  | 44:V:37:ILE:N     | 2.16                     | 0.61              |
| 50:3:245:U:O2'    | 50:3:246:A:H5'    | 2.01                     | 0.61              |
| 50:3:1084:G:H5'   | 50:3:1102:A:OP2   | 2.01                     | 0.61              |
| 2:c:2:ILE:HD11    | 2:c:48:ILE:HD11   | 1.82                     | 0.61              |
| 3:d:69:ARG:HH12   | 51:1:2060:A:H62   | 1.47                     | 0.61              |
| 9:l:77:ILE:HD12   | 9:l:77:ILE:N      | 2.15                     | 0.61              |
| 10:m:20:LEU:HG    | 19:v:81:PRO:HG2   | 1.82                     | 0.61              |
| 37:O:40:ILE:HD12  | 37:O:73:LEU:CB    | 2.31                     | 0.61              |
| 41:S:65:GLN:HB2   | 41:S:78:LEU:HD22  | 1.82                     | 0.61              |
| 49:a:7:ARG:HH12   | 49:a:218:MET:HB3  | 1.65                     | 0.61              |
| 49:a:173:THR:HG22 | 49:a:174:THR:H    | 1.65                     | 0.61              |
| 51:1:669:G:H2'    | 51:1:669:G:N3     | 2.16                     | 0.61              |
| 7:j:24:THR:CG2    | 7:j:27:ARG:HB2    | 2.31                     | 0.60              |
| 29:G:22:TRP:HE1   | 50:3:830:G:H5'    | 1.66                     | 0.60              |
| 29:G:63:LYS:HA    | 29:G:224:ARG:HH22 | 1.66                     | 0.60              |
| 37:O:42:LEU:HD11  | 37:O:73:LEU:HG    | 1.82                     | 0.60              |
| 50:3:1034:G:H2'   | 50:3:1035:A:H5'   | 1.82                     | 0.60              |
| 51:1:119:A:H4'    | 51:1:120:U:H5'    | 1.82                     | 0.60              |
| 51:1:2179:C:H2'   | 51:1:2180:U:C5    | 2.35                     | 0.60              |
| 30:H:112:ALA:O    | 30:H:115:VAL:HG12 | 2.01                     | 0.60              |
| 31:I:6:PRO:HA     | 50:3:430:A:O5'    | 2.00                     | 0.60              |
| 31:I:164:ARG:HH11 | 31:I:164:ARG:HG3  | 1.64                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:K:35:LYS:O     | 33:K:64:VAL:HG23  | 2.01                     | 0.60              |
| 50:3:208:U:H2'    | 50:3:210:C:H1'    | 1.83                     | 0.60              |
| 50:3:211:G:C2'    | 50:3:212:G:H5'    | 2.32                     | 0.60              |
| 51:1:1367:A:C2'   | 51:1:1368:G:H5'   | 2.31                     | 0.60              |
| 55:8:33:ARG:O     | 55:8:37:VAL:HG23  | 2.00                     | 0.60              |
| 55:8:167:GLU:HB3  | 55:8:180:THR:HG22 | 1.83                     | 0.60              |
| 38:P:62:ALA:HB3   | 38:P:94:SER:OG    | 2.01                     | 0.60              |
| 45:W:31:TYR:CD2   | 45:W:54:LEU:HD21  | 2.36                     | 0.60              |
| 3:d:145:ASP:HB3   | 3:d:184:ASP:OD2   | 2.01                     | 0.60              |
| 33:K:90:MET:HE3   | 45:W:60:ARG:HD3   | 1.82                     | 0.60              |
| 42:T:31:LEU:O     | 42:T:35:ILE:HG13  | 2.00                     | 0.60              |
| 46:X:2:ARG:HG2    | 50:3:1312:G:N7    | 2.16                     | 0.60              |
| 4:e:101:ARG:HA    | 4:e:105:ILE:HD11  | 1.83                     | 0.60              |
| 14:q:80:ASN:OD1   | 51:1:1151:A:H4'   | 2.01                     | 0.60              |
| 18:u:35:VAL:HG11  | 18:u:38:ILE:HB    | 1.83                     | 0.60              |
| 25:C:24:LYS:HG2   | 25:C:25:ASN:H     | 1.66                     | 0.60              |
| 43:U:68:SER:HB3   | 43:U:71:VAL:HG22  | 1.82                     | 0.60              |
| 6:g:126:GLY:O     | 6:g:146:VAL:HG12  | 2.01                     | 0.60              |
| 29:G:96:LEU:HG    | 50:3:1103:C:H4'   | 1.84                     | 0.60              |
| 44:V:61:ARG:HB3   | 44:V:61:ARG:NH1   | 2.15                     | 0.60              |
| 45:W:47:ARG:HB2   | 45:W:50:TYR:HD2   | 1.67                     | 0.60              |
| 50:3:505:G:H5'    | 50:3:534:U:H2'    | 1.83                     | 0.60              |
| 50:3:1094:G:N3    | 50:3:1094:G:H2'   | 2.17                     | 0.60              |
| 52:2:12:C:C2'     | 52:2:13:G:H4'     | 2.31                     | 0.60              |
| 16:s:69:LEU:HG    | 16:s:107:VAL:HG22 | 1.82                     | 0.60              |
| 36:N:91:GLU:OE1   | 36:N:94:ARG:HB2   | 2.02                     | 0.60              |
| 39:Q:98:ARG:NH1   | 39:Q:106:VAL:HG12 | 2.16                     | 0.60              |
| 50:3:1252:A:H61   | 50:3:1285:A:H61   | 1.49                     | 0.60              |
| 55:8:324:ARG:HH21 | 55:8:356:PHE:HB3  | 1.66                     | 0.60              |
| 4:e:124:ARG:HG3   | 4:e:160:LYS:HA    | 1.83                     | 0.60              |
| 10:m:76:LYS:HG2   | 10:m:80:VAL:HG11  | 1.82                     | 0.60              |
| 36:N:112:ARG:HD2  | 41:S:100:TRP:CD1  | 2.36                     | 0.60              |
| 47:Y:70:LYS:HA    | 47:Y:73:ARG:HH12  | 1.65                     | 0.60              |
| 51:1:69:C:O2'     | 51:1:70:G:H5'     | 2.02                     | 0.60              |
| 51:1:85:G:H3'     | 51:1:86:G:H5''    | 1.84                     | 0.60              |
| 51:1:441:U:O2'    | 51:1:442:G:H5'    | 2.01                     | 0.60              |
| 51:1:1073:A:C2'   | 51:1:1074:G:H5'   | 2.31                     | 0.60              |
| 51:1:2738:A:H61   | 51:1:2766:A:H61   | 1.50                     | 0.60              |
| 30:H:194:VAL:HG23 | 50:3:1205:U:H1'   | 1.83                     | 0.60              |
| 33:K:3:HIS:HB2    | 33:K:92:THR:HA    | 1.82                     | 0.60              |
| 46:X:62:THR:OG1   | 46:X:65:MET:HG2   | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 48:Z:48:LYS:O    | 48:Z:52:VAL:HG23 | 2.01                     | 0.60              |
| 50:3:1261:A:H5'' | 50:3:1262:C:H5   | 1.66                     | 0.60              |
| 51:1:2093:G:N7   | 51:1:2225:A:H2'  | 2.17                     | 0.60              |
| 51:1:2585:U:P    | 55:8:249:ALA:HB2 | 2.41                     | 0.60              |
| 51:1:2646:C:H2'  | 51:1:2647:U:O4'  | 2.02                     | 0.60              |
| 55:8:49:GLU:HA   | 55:8:52:ARG:HD3  | 1.83                     | 0.60              |
| 6:g:50:ARG:O     | 6:g:54:LEU:N     | 2.34                     | 0.60              |
| 50:3:769:G:H4'   | 50:3:1513:A:H4'  | 1.84                     | 0.60              |
| 51:1:876:C:C2'   | 51:1:877:A:H5'   | 2.30                     | 0.60              |
| 2:c:62:LYS:N     | 2:c:63:PRO:HD2   | 2.17                     | 0.59              |
| 13:p:52:ARG:NH2  | 51:1:2720:U:H5'' | 2.16                     | 0.59              |
| 50:3:77:A:H2     | 50:3:92:U:H3     | 1.50                     | 0.59              |
| 51:1:1213:A:N6   | 51:1:1236:G:H1'  | 2.17                     | 0.59              |
| 4:e:103:ILE:HA   | 4:e:107:VAL:HG23 | 1.84                     | 0.59              |
| 26:D:34:ARG:HD2  | 26:D:39:ARG:HD2  | 1.82                     | 0.59              |
| 29:G:35:ASN:HB3  | 29:G:37:VAL:HG23 | 1.84                     | 0.59              |
| 33:K:1:MET:H2    | 33:K:65:GLU:HG2  | 1.66                     | 0.59              |
| 37:O:19:ASP:OD2  | 50:3:1152:A:H4'  | 2.02                     | 0.59              |
| 40:R:22:TYR:HD2  | 40:R:65:GLU:HG3  | 1.67                     | 0.59              |
| 51:1:9:G:H22     | 51:1:2629:U:H2'  | 1.68                     | 0.59              |
| 51:1:215:G:C4'   | 51:1:216:A:H4'   | 2.31                     | 0.59              |
| 51:1:445:C:H2'   | 51:1:446:G:O4'   | 2.02                     | 0.59              |
| 51:1:2106:U:H2'  | 51:1:2107:G:C8   | 2.37                     | 0.59              |
| 51:1:2244:U:H3'  | 51:1:2245:U:C5'  | 2.23                     | 0.59              |
| 2:c:24:VAL:HG21  | 2:c:188:LEU:HB3  | 1.85                     | 0.59              |
| 12:o:76:LYS:HD2  | 12:o:77:ALA:N    | 2.17                     | 0.59              |
| 44:V:29:LYS:HB2  | 44:V:36:PHE:CE1  | 2.37                     | 0.59              |
| 50:3:1496:C:H1'  | 50:3:1517:G:H22  | 1.67                     | 0.59              |
| 51:1:784:G:O2'   | 51:1:785:G:H8    | 1.85                     | 0.59              |
| 51:1:1846:G:H2'  | 51:1:1847:A:H4'  | 1.84                     | 0.59              |
| 51:1:1900:A:O4'  | 51:1:1970:A:H5'' | 2.02                     | 0.59              |
| 16:s:69:LEU:HA   | 16:s:109:ASP:HA  | 1.84                     | 0.59              |
| 35:M:63:LYS:HE3  | 35:M:70:VAL:HG11 | 1.84                     | 0.59              |
| 36:N:35:GLU:HA   | 36:N:39:GLY:HA3  | 1.84                     | 0.59              |
| 43:U:1:MET:HE2   | 43:U:66:THR:HG21 | 1.85                     | 0.59              |
| 51:1:279:A:H2'   | 51:1:280:U:H5'   | 1.85                     | 0.59              |
| 1:b:77:VAL:HG23  | 1:b:112:GLY:H    | 1.66                     | 0.59              |
| 3:d:21:ARG:HG2   | 3:d:110:SER:OG   | 2.03                     | 0.59              |
| 32:J:91:SER:OG   | 32:J:138:ALA:HB2 | 2.03                     | 0.59              |
| 36:N:64:ILE:HD13 | 36:N:78:ILE:HG23 | 1.84                     | 0.59              |
| 51:1:1417:C:H2'  | 51:1:1418:G:C8   | 2.38                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:1:2298:A:H62   | 51:1:2318:G:H21   | 1.50                     | 0.59              |
| 8:k:110:GLU:HA    | 8:k:113:MET:HG2   | 1.84                     | 0.59              |
| 31:I:149:LYS:HA   | 31:I:177:MET:HE1  | 1.85                     | 0.59              |
| 33:K:5:GLU:OE1    | 33:K:90:MET:HB2   | 2.02                     | 0.59              |
| 46:X:11:ASP:HB2   | 46:X:14:LEU:HB3   | 1.83                     | 0.59              |
| 46:X:18:VAL:O     | 46:X:22:VAL:HG22  | 2.03                     | 0.59              |
| 51:1:1856:U:H2'   | 51:1:1857:G:O4'   | 2.02                     | 0.59              |
| 7:j:1:MET:HE1     | 15:r:13:ARG:N     | 2.17                     | 0.59              |
| 17:t:13:ALA:HB1   | 22:y:33:ALA:HB2   | 1.85                     | 0.59              |
| 50:3:1296:C:H4'   | 50:3:1302:C:H42   | 1.68                     | 0.59              |
| 51:1:388:G:H2'    | 51:1:390:U:H5     | 1.67                     | 0.59              |
| 51:1:1111:A:O2'   | 51:1:1112:G:H4'   | 2.02                     | 0.59              |
| 6:g:76:GLU:OE2    | 6:g:142:VAL:HA    | 2.01                     | 0.59              |
| 27:E:39:ARG:NH1   | 51:1:2362:C:H5''  | 2.17                     | 0.59              |
| 28:F:32:LYS:HG2   | 51:1:2478:A:OP1   | 2.02                     | 0.59              |
| 29:G:116:LEU:CD1  | 29:G:143:LEU:HD12 | 2.33                     | 0.59              |
| 51:1:2285:C:O2'   | 51:1:2287:A:H1'   | 2.03                     | 0.59              |
| 1:b:62:ARG:HD3    | 1:b:83:ASP:OD1    | 2.03                     | 0.59              |
| 6:g:3:VAL:HA      | 6:g:39:ALA:H      | 1.67                     | 0.59              |
| 12:o:74:VAL:HA    | 12:o:77:ALA:HB3   | 1.85                     | 0.59              |
| 36:N:27:ILE:N     | 36:N:27:ILE:HD12  | 2.18                     | 0.59              |
| 36:N:45:MET:HA    | 36:N:48:ARG:HE    | 1.68                     | 0.59              |
| 37:O:48:ARG:NH1   | 50:3:1368:A:H4'   | 2.18                     | 0.59              |
| 51:1:554:U:H2'    | 51:1:555:G:O4'    | 2.02                     | 0.59              |
| 51:1:1043:C:C2'   | 51:1:1044:C:H5'   | 2.31                     | 0.59              |
| 9:l:63:LYS:HA     | 27:E:12:ARG:HG2   | 1.84                     | 0.58              |
| 11:n:29:VAL:HG21  | 11:n:75:ILE:HG23  | 1.85                     | 0.58              |
| 39:Q:54:VAL:N     | 39:Q:62:VAL:O     | 2.31                     | 0.58              |
| 46:X:38:THR:HA    | 46:X:69:LYS:HA    | 1.85                     | 0.58              |
| 51:1:955:U:H3     | 51:1:962:G:H1     | 1.48                     | 0.58              |
| 52:2:88:C:OP1     | 52:2:88:C:H3'     | 2.03                     | 0.58              |
| 2:c:48:ILE:O      | 2:c:81:GLU:HG3    | 2.02                     | 0.58              |
| 13:p:103:THR:HA   | 13:p:107:ALA:HB2  | 1.84                     | 0.58              |
| 16:s:42:LYS:CB    | 51:1:2010:G:H5''  | 2.32                     | 0.58              |
| 30:H:112:ALA:HB3  | 30:H:184:ASN:ND2  | 2.18                     | 0.58              |
| 30:H:148:ILE:HG13 | 30:H:169:GLU:HB3  | 1.85                     | 0.58              |
| 30:H:156:LEU:HD12 | 30:H:156:LEU:O    | 2.03                     | 0.58              |
| 31:I:143:SER:HB2  | 31:I:178:GLU:HG2  | 1.85                     | 0.58              |
| 33:K:3:HIS:N      | 33:K:92:THR:HG22  | 2.17                     | 0.58              |
| 41:S:79:SER:HB3   | 41:S:82:LYS:CG    | 2.33                     | 0.58              |
| 51:1:362:A:H3'    | 51:1:363:G:H8     | 1.68                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 51:1:2156:G:H2'  | 51:1:2157:G:H5'   | 1.86                     | 0.58              |
| 5:f:2:ARG:HB2    | 51:1:2751:G:O4'   | 2.02                     | 0.58              |
| 32:J:160:VAL:O   | 32:J:164:LEU:HG   | 2.03                     | 0.58              |
| 41:S:13:VAL:HA   | 41:S:16:ALA:HB3   | 1.85                     | 0.58              |
| 51:1:1869:G:H2'  | 51:1:1871:A:OP1   | 2.02                     | 0.58              |
| 51:1:2259:U:O2   | 51:1:2259:U:H2'   | 2.02                     | 0.58              |
| 51:1:2834:G:H2'  | 51:1:2879:A:H61   | 1.68                     | 0.58              |
| 4:e:25:MET:HB3   | 52:2:57:A:C2      | 2.38                     | 0.58              |
| 29:G:39:ILE:HD12 | 29:G:39:ILE:N     | 2.17                     | 0.58              |
| 34:L:12:LEU:HD12 | 34:L:13:PRO:HD2   | 1.84                     | 0.58              |
| 39:Q:109:ARG:HB3 | 39:Q:118:VAL:HG21 | 1.85                     | 0.58              |
| 43:U:14:ARG:HE   | 43:U:42:ILE:HD12  | 1.69                     | 0.58              |
| 50:3:846:G:H2'   | 50:3:846:G:N3     | 2.17                     | 0.58              |
| 50:3:1241:G:H2'  | 50:3:1242:G:H8    | 1.67                     | 0.58              |
| 51:1:227:A:H2'   | 51:1:228:C:H4'    | 1.86                     | 0.58              |
| 21:x:32:LEU:HA   | 21:x:51:SER:HA    | 1.86                     | 0.58              |
| 22:y:2:LYS:HD2   | 51:1:78:U:OP2     | 2.02                     | 0.58              |
| 31:I:25:ARG:HD2  | 50:3:410:G:OP1    | 2.04                     | 0.58              |
| 34:L:115:MET:HG2 | 50:3:1240:U:OP1   | 2.03                     | 0.58              |
| 35:M:120:LEU:HA  | 50:3:600:A:H5'    | 1.85                     | 0.58              |
| 51:1:1827:U:O2'  | 51:1:1828:G:H5'   | 2.04                     | 0.58              |
| 8:k:6:THR:HG23   | 51:1:1666:G:H4'   | 1.86                     | 0.58              |
| 18:u:39:ASN:HB3  | 18:u:62:ALA:HB3   | 1.84                     | 0.58              |
| 31:I:121:ALA:C   | 31:I:122:ILE:HD12 | 2.28                     | 0.58              |
| 50:3:1447:A:H5'' | 50:3:1448:C:H5    | 1.67                     | 0.58              |
| 2:c:142:VAL:CG2  | 2:c:143:PRO:HD2   | 2.34                     | 0.58              |
| 4:e:147:ARG:HD3  | 4:e:148:VAL:N     | 2.19                     | 0.58              |
| 14:q:107:ALA:HB3 | 15:r:48:LYS:HZ1   | 1.64                     | 0.58              |
| 23:z:23:LEU:HD11 | 23:z:53:MET:SD    | 2.44                     | 0.58              |
| 29:G:122:ASP:OD1 | 29:G:124:THR:HG23 | 2.03                     | 0.58              |
| 34:L:137:ARG:HD2 | 34:L:137:ARG:C    | 2.29                     | 0.58              |
| 49:a:204:ALA:HB3 | 51:1:1861:G:OP1   | 2.03                     | 0.58              |
| 50:3:1457:G:H2'  | 50:3:1458:G:H8    | 1.68                     | 0.58              |
| 51:1:1418:G:H21  | 51:1:1580:A:H62   | 1.52                     | 0.58              |
| 51:1:1422:G:H1'  | 51:1:1496:A:H61   | 1.68                     | 0.58              |
| 51:1:2860:A:H2'  | 51:1:2861:U:H5'   | 1.85                     | 0.58              |
| 4:e:82:TYR:O     | 4:e:84:ILE:HG12   | 2.03                     | 0.58              |
| 14:q:5:ARG:NH1   | 51:1:585:G:N7     | 2.52                     | 0.58              |
| 17:t:68:LYS:HB2  | 17:t:77:ARG:HH12  | 1.69                     | 0.58              |
| 19:v:38:LEU:HD23 | 19:v:40:ILE:HD11  | 1.86                     | 0.58              |
| 22:y:42:LEU:O    | 22:y:46:VAL:HG23  | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:I:8:LEU:N      | 50:3:430:A:OP1    | 2.36                     | 0.58              |
| 32:J:108:GLY:O    | 32:J:109:ALA:HB3  | 2.04                     | 0.58              |
| 50:3:1305:G:N2    | 50:3:1331:G:H2'   | 2.18                     | 0.58              |
| 7:j:25:LEU:HB3    | 51:1:1140:C:OP1   | 2.04                     | 0.58              |
| 13:p:55:HIS:NE2   | 51:1:2682:A:H4'   | 2.18                     | 0.58              |
| 29:G:220:VAL:O    | 29:G:224:ARG:HG2  | 2.03                     | 0.58              |
| 33:K:11:HIS:ND1   | 33:K:12:PRO:HD2   | 2.19                     | 0.58              |
| 51:1:1954:G:H21   | 51:1:1956:U:H3    | 1.50                     | 0.58              |
| 15:r:49:ILE:HG22  | 15:r:54:VAL:CG1   | 2.33                     | 0.58              |
| 34:L:113:LYS:HB3  | 50:3:1297:G:H21   | 1.69                     | 0.58              |
| 50:3:12:U:H4'     | 50:3:526:C:H4'    | 1.84                     | 0.58              |
| 20:w:22:PHE:HD2   | 51:1:922:C:H1'    | 1.69                     | 0.57              |
| 31:I:49:ASP:O     | 31:I:52:VAL:HG12  | 2.04                     | 0.57              |
| 34:L:20:GLU:HA    | 34:L:23:ALA:HB3   | 1.86                     | 0.57              |
| 39:Q:5:GLN:HE21   | 50:3:880:C:H3'    | 1.68                     | 0.57              |
| 48:Z:16:ARG:HD2   | 48:Z:18:PHE:HB3   | 1.85                     | 0.57              |
| 51:1:1744:A:H3'   | 51:1:1745:A:C8    | 2.39                     | 0.57              |
| 51:1:2163:A:H2'   | 51:1:2164:C:H5'   | 1.86                     | 0.57              |
| 2:c:55:LYS:HE2    | 2:c:59:ARG:HB3    | 1.86                     | 0.57              |
| 5:f:68:ARG:HD3    | 5:f:68:ARG:C      | 2.30                     | 0.57              |
| 24:B:45:ASP:OD2   | 24:B:47:TYR:HD2   | 1.88                     | 0.57              |
| 31:I:120:LYS:HZ1  | 50:3:439:U:H5''   | 1.69                     | 0.57              |
| 33:K:66:ALA:HB1   | 33:K:67:PRO:HD2   | 1.85                     | 0.57              |
| 50:3:1413:A:H2    | 50:3:1487:G:H22   | 1.50                     | 0.57              |
| 51:1:275:C:H2'    | 51:1:276:U:H4'    | 1.86                     | 0.57              |
| 51:1:1821:A:H2'   | 51:1:1822:C:C6    | 2.39                     | 0.57              |
| 55:8:117:ARG:HH12 | 55:8:357:ILE:HG22 | 1.69                     | 0.57              |
| 55:8:144:TRP:HH2  | 55:8:199:HIS:C    | 2.12                     | 0.57              |
| 3:d:3:LEU:HB2     | 3:d:12:LEU:HB3    | 1.87                     | 0.57              |
| 25:C:3:GLY:HA3    | 51:1:2283:C:O3'   | 2.04                     | 0.57              |
| 30:H:19:SER:O     | 41:S:93:PRO:HG3   | 2.04                     | 0.57              |
| 33:K:45:ARG:HG2   | 33:K:59:TYR:CD2   | 2.39                     | 0.57              |
| 51:1:1344:U:H3'   | 51:1:1345:C:H5'   | 1.86                     | 0.57              |
| 51:1:1837:C:H2'   | 51:1:1899:A:H61   | 1.68                     | 0.57              |
| 51:1:2600:A:O2'   | 51:1:2601:C:H5'   | 2.04                     | 0.57              |
| 7:j:27:ARG:HH22   | 51:1:1142:A:H4'   | 1.70                     | 0.57              |
| 29:G:104:LYS:HA   | 29:G:107:ARG:NH1  | 2.19                     | 0.57              |
| 35:M:36:ALA:O     | 35:M:45:ILE:HD11  | 2.04                     | 0.57              |
| 43:U:19:VAL:HG12  | 43:U:37:GLY:C     | 2.30                     | 0.57              |
| 50:3:1256:A:H1'   | 50:3:1258:G:N9    | 2.19                     | 0.57              |
| 51:1:727:A:O2'    | 51:1:728:G:H5'    | 2.05                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 51:1:783:A:H8    | 51:1:784:G:H4'   | 1.69                     | 0.57              |
| 51:1:2451:A:H4'  | 55:8:256:ARG:NH1 | 2.19                     | 0.57              |
| 1:b:48:ILE:HD11  | 1:b:51:ARG:HA    | 1.85                     | 0.57              |
| 15:r:34:GLU:OE1  | 15:r:60:LYS:HG2  | 2.04                     | 0.57              |
| 18:u:48:VAL:HG22 | 18:u:52:ASN:HB3  | 1.85                     | 0.57              |
| 41:S:5:MET:HE3   | 41:S:62:ARG:NH2  | 2.18                     | 0.57              |
| 51:1:85:G:C2'    | 51:1:86:G:H5''   | 2.34                     | 0.57              |
| 1:b:19:VAL:HG22  | 1:b:20:ASN:N     | 2.19                     | 0.57              |
| 4:e:37:MET:HB2   | 4:e:86:CYS:HB2   | 1.87                     | 0.57              |
| 9:l:60:ARG:NH2   | 51:1:2428:G:H21  | 2.02                     | 0.57              |
| 25:C:22:THR:HG22 | 25:C:23:THR:N    | 2.16                     | 0.57              |
| 34:L:112:ASP:OD2 | 34:L:121:ASN:ND2 | 2.38                     | 0.57              |
| 51:1:466:A:H2'   | 51:1:467:G:H5'   | 1.85                     | 0.57              |
| 51:1:2193:G:H2'  | 51:1:2194:U:C6   | 2.38                     | 0.57              |
| 1:b:16:VAL:HB    | 1:b:203:VAL:HG12 | 1.86                     | 0.57              |
| 23:z:35:VAL:HG22 | 23:z:37:ARG:NH1  | 2.20                     | 0.57              |
| 34:L:79:VAL:HG23 | 34:L:80:GLY:H    | 1.70                     | 0.57              |
| 35:M:10:LEU:HD22 | 35:M:74:ILE:HD11 | 1.85                     | 0.57              |
| 40:R:53:ASP:N    | 40:R:56:ARG:HH21 | 2.01                     | 0.57              |
| 41:S:29:ILE:CG1  | 41:S:30:ILE:HD12 | 2.33                     | 0.57              |
| 42:T:23:SER:HB3  | 42:T:26:VAL:HG23 | 1.86                     | 0.57              |
| 50:3:1486:G:H2'  | 50:3:1487:G:C8   | 2.40                     | 0.57              |
| 51:1:1645:G:H5'' | 51:1:1646:C:C5'  | 2.24                     | 0.57              |
| 4:e:95:MET:HE3   | 4:e:96:TRP:NE1   | 2.20                     | 0.57              |
| 4:e:103:ILE:HA   | 4:e:107:VAL:CG2  | 2.35                     | 0.57              |
| 14:q:23:TYR:HD1  | 51:1:533:G:H5'   | 1.68                     | 0.57              |
| 17:t:11:LEU:HD23 | 17:t:12:ARG:N    | 2.19                     | 0.57              |
| 24:B:14:MET:SD   | 51:1:2045:C:H5'' | 2.44                     | 0.57              |
| 40:R:96:VAL:HG22 | 50:3:1308:U:OP1  | 2.04                     | 0.57              |
| 42:T:2:LEU:HD13  | 42:T:34:GLN:OE1  | 2.04                     | 0.57              |
| 43:U:33:ILE:HD12 | 43:U:33:ILE:H    | 1.70                     | 0.57              |
| 54:4:22:A:OP2    | 55:8:212:ARG:HD2 | 2.05                     | 0.57              |
| 55:8:120:SER:HB3 | 55:8:193:ARG:NH2 | 2.13                     | 0.57              |
| 4:e:65:LEU:HD22  | 52:2:42:C:C6     | 2.40                     | 0.57              |
| 51:1:948:C:H2'   | 51:1:949:G:C8    | 2.40                     | 0.57              |
| 1:b:229:HIS:ND1  | 1:b:230:PRO:HD2  | 2.19                     | 0.57              |
| 4:e:103:ILE:HG22 | 4:e:107:VAL:HG21 | 1.86                     | 0.57              |
| 5:f:152:ARG:HG3  | 5:f:153:PRO:HD2  | 1.85                     | 0.57              |
| 8:k:40:LYS:HE3   | 8:k:57:VAL:HG12  | 1.87                     | 0.57              |
| 12:o:56:LYS:O    | 12:o:60:GLU:HG2  | 2.05                     | 0.57              |
| 17:t:87:LEU:H    | 17:t:87:LEU:HD12 | 1.68                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:H:19:SER:HB3   | 30:H:21:TRP:HE1   | 1.70                     | 0.57              |
| 33:K:6:ILE:HB     | 33:K:62:MET:HB2   | 1.87                     | 0.57              |
| 33:K:18:VAL:N     | 33:K:19:PRO:CD    | 2.67                     | 0.57              |
| 34:L:28:ILE:HG21  | 34:L:104:VAL:HG21 | 1.87                     | 0.57              |
| 43:U:51:ARG:C     | 43:U:52:LEU:HD12  | 2.30                     | 0.57              |
| 44:V:15:LYS:HE3   | 50:3:275:G:C5'    | 2.34                     | 0.57              |
| 51:1:114:U:H6     | 51:1:114:U:H5'    | 1.69                     | 0.57              |
| 1:b:143:VAL:HG22  | 1:b:189:ALA:CB    | 2.34                     | 0.56              |
| 2:c:135:GLY:HA2   | 51:1:743:A:OP1    | 2.05                     | 0.56              |
| 8:k:2:ILE:HB      | 8:k:33:ALA:HB3    | 1.85                     | 0.56              |
| 12:o:15:ARG:NH2   | 52:2:8:C:H5''     | 2.19                     | 0.56              |
| 13:p:30:TRP:CE2   | 13:p:37:LYS:HG2   | 2.40                     | 0.56              |
| 25:C:9:LYS:HE3    | 25:C:19:PHE:CD2   | 2.39                     | 0.56              |
| 34:L:137:ARG:O    | 34:L:140:VAL:HG12 | 2.04                     | 0.56              |
| 38:P:110:THR:HG22 | 48:Z:4:LYS:HG3    | 1.86                     | 0.56              |
| 50:3:252:U:O2     | 50:3:252:U:H2'    | 2.05                     | 0.56              |
| 51:1:655:A:H4'    | 51:1:656:G:H5'    | 1.86                     | 0.56              |
| 3:d:127:GLU:H     | 3:d:127:GLU:CD    | 2.13                     | 0.56              |
| 5:f:26:LYS:HD2    | 5:f:31:GLU:HB3    | 1.86                     | 0.56              |
| 6:g:58:LEU:HA     | 6:g:61:VAL:HG23   | 1.87                     | 0.56              |
| 12:o:89:ASP:HA    | 12:o:116:GLN:HB2  | 1.87                     | 0.56              |
| 17:t:87:LEU:HD12  | 17:t:87:LEU:N     | 2.20                     | 0.56              |
| 21:x:17:ARG:HH21  | 21:x:21:LEU:HD22  | 1.69                     | 0.56              |
| 35:M:7:ALA:HB2    | 35:M:76:ARG:HH11  | 1.71                     | 0.56              |
| 36:N:115:VAL:HG13 | 37:O:62:ARG:HH11  | 1.68                     | 0.56              |
| 38:P:52:ARG:HH22  | 38:P:56:LYS:HD3   | 1.69                     | 0.56              |
| 41:S:45:LEU:HG    | 46:X:12:LEU:HD13  | 1.87                     | 0.56              |
| 43:U:71:VAL:O     | 43:U:75:ILE:HG13  | 2.04                     | 0.56              |
| 44:V:11:VAL:CG1   | 44:V:20:ILE:HD11  | 2.35                     | 0.56              |
| 47:Y:79:THR:O     | 47:Y:82:ILE:HG12  | 2.05                     | 0.56              |
| 51:1:875:G:H1     | 51:1:902:C:H42    | 1.53                     | 0.56              |
| 4:e:63:LYS:HG3    | 52:2:42:C:H4'     | 1.87                     | 0.56              |
| 6:g:63:ALA:HA     | 6:g:66:ASN:HD21   | 1.71                     | 0.56              |
| 6:g:103:VAL:CG1   | 6:g:108:VAL:HB    | 2.32                     | 0.56              |
| 9:l:51:GLU:HB2    | 51:1:833:A:H1'    | 1.87                     | 0.56              |
| 11:n:2:ARG:O      | 11:n:2:ARG:HD3    | 2.05                     | 0.56              |
| 30:H:9:ILE:HG23   | 30:H:10:ARG:HG3   | 1.87                     | 0.56              |
| 30:H:27:GLU:O     | 30:H:31:ASN:ND2   | 2.39                     | 0.56              |
| 30:H:149:LYS:HB3  | 30:H:200:TRP:HB2  | 1.87                     | 0.56              |
| 32:J:25:LYS:HG2   | 50:3:923:A:OP1    | 2.05                     | 0.56              |
| 33:K:1:MET:N      | 33:K:65:GLU:HG2   | 2.21                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 33:K:91:ARG:HH21 | 45:W:56:ARG:HE   | 1.52                     | 0.56              |
| 36:N:11:ARG:HH12 | 36:N:108:ARG:HD2 | 1.71                     | 0.56              |
| 38:P:38:GLY:O    | 50:3:683:G:N2    | 2.38                     | 0.56              |
| 41:S:9:GLU:OE1   | 41:S:62:ARG:HG3  | 2.06                     | 0.56              |
| 41:S:60:ARG:NH1  | 50:3:981:U:H1'   | 2.21                     | 0.56              |
| 43:U:8:ARG:HG2   | 43:U:8:ARG:HH11  | 1.71                     | 0.56              |
| 49:a:197:LYS:NZ  | 51:1:1873:G:N3   | 2.54                     | 0.56              |
| 50:3:1024:G:C2'  | 50:3:1025:U:H5'  | 2.36                     | 0.56              |
| 51:1:703:U:H2'   | 51:1:704:G:O4'   | 2.05                     | 0.56              |
| 51:1:1326:U:H2'  | 51:1:1327:A:H8   | 1.70                     | 0.56              |
| 54:4:21:A:H2'    | 55:8:214:HIS:CD2 | 2.39                     | 0.56              |
| 55:8:358:GLU:O   | 55:8:362:LYS:HB2 | 2.05                     | 0.56              |
| 3:d:109:LEU:HD23 | 3:d:112:LEU:HD12 | 1.88                     | 0.56              |
| 6:g:84:ALA:HB3   | 6:g:148:ALA:HB2  | 1.88                     | 0.56              |
| 51:1:1872:A:H2'  | 51:1:1873:G:O4'  | 2.05                     | 0.56              |
| 55:8:265:HIS:O   | 55:8:269:GLY:N   | 2.38                     | 0.56              |
| 4:e:47:LYS:HA    | 4:e:50:ASP:OD2   | 2.05                     | 0.56              |
| 32:J:53:ARG:HG2  | 32:J:53:ARG:HH11 | 1.70                     | 0.56              |
| 34:L:137:ARG:HD2 | 34:L:137:ARG:O   | 2.05                     | 0.56              |
| 44:V:16:MET:SD   | 44:V:21:VAL:HG13 | 2.45                     | 0.56              |
| 48:Z:31:VAL:O    | 48:Z:31:VAL:HG22 | 2.05                     | 0.56              |
| 50:3:517:G:O2'   | 50:3:530:G:H5''  | 2.05                     | 0.56              |
| 51:1:133:U:H2'   | 51:1:134:G:C8    | 2.40                     | 0.56              |
| 51:1:1991:U:H2'  | 51:1:1992:G:H5'' | 1.88                     | 0.56              |
| 51:1:2469:A:H2'  | 51:1:2470:G:O4'  | 2.05                     | 0.56              |
| 51:1:2529:G:H5'' | 51:1:2530:A:H5'' | 1.87                     | 0.56              |
| 54:4:19:U:N3     | 55:8:137:GLY:O   | 2.39                     | 0.56              |
| 1:b:28:PRO:CG    | 1:b:33:LEU:HD21  | 2.36                     | 0.56              |
| 15:r:79:ARG:HD2  | 15:r:80:ARG:HH12 | 1.71                     | 0.56              |
| 49:a:205:LYS:CA  | 51:1:1860:G:H4'  | 2.31                     | 0.56              |
| 5:f:21:GLN:NE2   | 5:f:38:ASP:HA    | 2.20                     | 0.56              |
| 12:o:7:ARG:HA    | 12:o:10:ARG:NH1  | 2.20                     | 0.56              |
| 31:I:54:LEU:HD12 | 31:I:57:LYS:HE2  | 1.86                     | 0.56              |
| 33:K:23:GLU:CA   | 33:K:26:THR:HG22 | 2.32                     | 0.56              |
| 38:P:95:THR:O    | 38:P:99:LEU:HG   | 2.05                     | 0.56              |
| 50:3:77:A:H2'    | 50:3:78:A:C8     | 2.41                     | 0.56              |
| 51:1:366:C:C3'   | 51:1:367:G:H5''  | 2.35                     | 0.56              |
| 5:f:155:PRO:O    | 5:f:171:LYS:N    | 2.39                     | 0.56              |
| 10:m:36:VAL:HG12 | 10:m:127:LYS:O   | 2.06                     | 0.56              |
| 17:t:44:LYS:HG3  | 17:t:55:VAL:HG21 | 1.87                     | 0.56              |
| 19:v:80:HIS:ND1  | 19:v:81:PRO:HD2  | 2.21                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:H:127:VAL:HG22 | 30:H:128:MET:H    | 1.70                     | 0.56              |
| 31:I:122:ILE:HD12 | 31:I:122:ILE:N    | 2.21                     | 0.56              |
| 38:P:123:PRO:C    | 38:P:124:LYS:HE2  | 2.31                     | 0.56              |
| 49:a:181:ASP:OD2  | 49:a:184:LYS:HG2  | 2.06                     | 0.56              |
| 50:3:1457:G:H2'   | 50:3:1458:G:C8    | 2.41                     | 0.56              |
| 3:d:149:ILE:HG21  | 3:d:188:MET:SD    | 2.46                     | 0.56              |
| 12:o:111:ARG:HG2  | 12:o:111:ARG:HH21 | 1.70                     | 0.56              |
| 13:p:47:ILE:HD11  | 13:p:61:ARG:N     | 2.21                     | 0.56              |
| 17:t:61:LEU:HD13  | 51:1:1341:G:H5'   | 1.87                     | 0.56              |
| 33:K:68:GLN:O     | 33:K:71:ILE:HG22  | 2.06                     | 0.56              |
| 35:M:115:ALA:O    | 35:M:119:GLY:N    | 2.37                     | 0.56              |
| 38:P:43:TRP:NE1   | 50:3:686:U:H4'    | 2.21                     | 0.56              |
| 38:P:127:ARG:HG3  | 48:Z:34:ARG:NH2   | 2.20                     | 0.56              |
| 4:e:39:VAL:HG12   | 4:e:41:GLU:H      | 1.70                     | 0.56              |
| 20:w:36:GLN:HE22  | 20:w:39:THR:HA    | 1.70                     | 0.56              |
| 29:G:133:ALA:O    | 29:G:137:THR:HG23 | 2.06                     | 0.56              |
| 33:K:12:PRO:HA    | 33:K:44:ARG:HD3   | 1.87                     | 0.56              |
| 33:K:48:ALA:HB1   | 45:W:68:PRO:HD3   | 1.88                     | 0.56              |
| 35:M:48:PHE:C     | 35:M:49:LYS:HD2   | 2.30                     | 0.56              |
| 55:8:11:ILE:CD1   | 55:8:80:VAL:HG21  | 2.36                     | 0.56              |
| 4:e:102:LEU:O     | 4:e:106:ALA:HB3   | 2.06                     | 0.55              |
| 7:j:13:ARG:HH21   | 7:j:13:ARG:HG2    | 1.70                     | 0.55              |
| 29:G:89:PHE:HB3   | 29:G:150:ILE:HG22 | 1.88                     | 0.55              |
| 33:K:21:MET:HG2   | 33:K:24:ARG:CZ    | 2.36                     | 0.55              |
| 50:3:1170:A:C2'   | 50:3:1171:A:H5'   | 2.35                     | 0.55              |
| 51:1:133:U:H2'    | 51:1:134:G:H8     | 1.71                     | 0.55              |
| 7:j:28:LEU:O      | 7:j:32:LEU:HD23   | 2.07                     | 0.55              |
| 30:H:86:LEU:O     | 30:H:90:VAL:HG22  | 2.06                     | 0.55              |
| 31:I:103:ARG:NH1  | 31:I:169:TRP:HH2  | 2.04                     | 0.55              |
| 34:L:28:ILE:HG22  | 34:L:104:VAL:HG21 | 1.88                     | 0.55              |
| 36:N:61:ASP:C     | 36:N:62:LEU:HD22  | 2.31                     | 0.55              |
| 39:Q:23:LEU:HD23  | 39:Q:29:LYS:HD3   | 1.88                     | 0.55              |
| 39:Q:27:PRO:C     | 39:Q:28:GLN:HG3   | 2.31                     | 0.55              |
| 46:X:39:ILE:HB    | 46:X:66:VAL:O     | 2.07                     | 0.55              |
| 46:X:54:ARG:HG2   | 46:X:54:ARG:HH11  | 1.71                     | 0.55              |
| 50:3:1071:C:H2'   | 50:3:1072:G:C8    | 2.40                     | 0.55              |
| 55:8:125:SER:HA   | 55:8:187:TYR:H    | 1.70                     | 0.55              |
| 3:d:9:GLN:H       | 3:d:9:GLN:CD      | 2.14                     | 0.55              |
| 9:l:91:ASP:HB2    | 9:l:92:LEU:HD23   | 1.87                     | 0.55              |
| 20:w:35:ARG:HH21  | 51:1:2355:G:H1'   | 1.72                     | 0.55              |
| 29:G:27:LYS:HB2   | 29:G:28:PRO:HD3   | 1.87                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 35:M:10:LEU:HD22  | 35:M:74:ILE:HD13 | 1.88                     | 0.55              |
| 36:N:11:ARG:HH22  | 36:N:108:ARG:HD2 | 1.72                     | 0.55              |
| 38:P:66:ALA:HB3   | 38:P:98:ALA:HB1  | 1.88                     | 0.55              |
| 39:Q:34:THR:OG1   | 39:Q:53:ARG:HD2  | 2.06                     | 0.55              |
| 39:Q:38:THR:HG21  | 39:Q:48:LEU:HB3  | 1.88                     | 0.55              |
| 41:S:20:PHE:O     | 41:S:21:ALA:HB3  | 2.07                     | 0.55              |
| 50:3:686:U:H2'    | 50:3:687:A:C8    | 2.42                     | 0.55              |
| 51:1:367:G:H2'    | 51:1:368:A:O4'   | 2.06                     | 0.55              |
| 51:1:940:G:C2'    | 51:1:941:A:H5''  | 2.36                     | 0.55              |
| 51:1:1437:C:H5''  | 51:1:1552:A:H61  | 1.71                     | 0.55              |
| 51:1:2208:C:H2'   | 51:1:2209:G:C8   | 2.42                     | 0.55              |
| 51:1:2254:C:H2'   | 51:1:2255:G:C8   | 2.42                     | 0.55              |
| 52:2:66:A:H4'     | 52:2:67:G:C8     | 2.41                     | 0.55              |
| 3:d:148:ILE:HB    | 3:d:169:VAL:HA   | 1.88                     | 0.55              |
| 8:k:49:ARG:NH2    | 50:3:1422:G:H4'  | 2.21                     | 0.55              |
| 31:I:78:ALA:HB2   | 31:I:89:LEU:HD21 | 1.86                     | 0.55              |
| 31:I:120:LYS:NZ   | 50:3:439:U:H5''  | 2.21                     | 0.55              |
| 35:M:80:PRO:HG2   | 50:3:878:A:C5'   | 2.36                     | 0.55              |
| 40:R:51:GLN:O     | 40:R:55:LEU:HD23 | 2.06                     | 0.55              |
| 44:V:24:ILE:CG2   | 44:V:41:THR:HB   | 2.37                     | 0.55              |
| 50:3:1118:U:H2'   | 50:3:1119:C:C6   | 2.41                     | 0.55              |
| 51:1:593:U:H2'    | 51:1:594:U:C6    | 2.42                     | 0.55              |
| 51:1:1494:A:H2'   | 51:1:1494:A:N3   | 2.22                     | 0.55              |
| 51:1:2484:G:O2'   | 51:1:2485:G:H5'  | 2.07                     | 0.55              |
| 3:d:194:LYS:O     | 3:d:198:GLU:HG2  | 2.06                     | 0.55              |
| 4:e:95:MET:HE3    | 4:e:96:TRP:HE1   | 1.72                     | 0.55              |
| 11:n:28:LEU:HD23  | 11:n:48:VAL:HG11 | 1.89                     | 0.55              |
| 11:n:39:PRO:HG2   | 51:1:1651:G:H4'  | 1.89                     | 0.55              |
| 34:L:111:GLY:CA   | 34:L:118:ARG:HD3 | 2.23                     | 0.55              |
| 37:O:8:ILE:HG13   | 37:O:98:VAL:HG13 | 1.89                     | 0.55              |
| 38:P:66:ALA:CB    | 38:P:98:ALA:HB3  | 2.35                     | 0.55              |
| 40:R:22:TYR:CE1   | 50:3:1330:U:H4'  | 2.42                     | 0.55              |
| 43:U:12:LYS:HG3   | 50:3:44:A:OP2    | 2.07                     | 0.55              |
| 44:V:58:VAL:HG12  | 44:V:77:VAL:HG13 | 1.87                     | 0.55              |
| 50:3:279:A:H5'    | 50:3:281:G:C5'   | 2.28                     | 0.55              |
| 50:3:673:A:H2'    | 50:3:674:G:C8    | 2.41                     | 0.55              |
| 51:1:479:A:H1'    | 51:1:481:G:H5''  | 1.88                     | 0.55              |
| 55:8:183:ILE:HD12 | 55:8:183:ILE:N   | 2.22                     | 0.55              |
| 1:b:209:ALA:O     | 1:b:213:ARG:HG3  | 2.06                     | 0.55              |
| 3:d:200:LEU:HD12  | 3:d:201:ALA:N    | 2.21                     | 0.55              |
| 4:e:107:VAL:N     | 4:e:108:PRO:CD   | 2.69                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:j:38:GLY:HA3    | 7:j:50:THR:HG23   | 1.89                     | 0.55              |
| 8:k:102:PRO:HD3   | 13:p:65:ASN:ND2   | 2.20                     | 0.55              |
| 9:l:123:ARG:O     | 9:l:125:LEU:HD13  | 2.06                     | 0.55              |
| 15:r:24:LYS:HA    | 15:r:94:THR:OG1   | 2.05                     | 0.55              |
| 29:G:117:GLU:O    | 29:G:121:GLN:HG2  | 2.06                     | 0.55              |
| 31:I:9:LYS:HE2    | 50:3:542:G:H5''   | 1.87                     | 0.55              |
| 34:L:1:PRO:HG3    | 50:3:1345:U:O4    | 2.07                     | 0.55              |
| 38:P:66:ALA:HB3   | 38:P:98:ALA:HB3   | 1.88                     | 0.55              |
| 42:T:63:ARG:HH22  | 42:T:87:ARG:HH12  | 1.54                     | 0.55              |
| 46:X:78:THR:HG23  | 50:3:957:U:H4'    | 1.87                     | 0.55              |
| 50:3:304:U:O2'    | 50:3:305:G:H5'    | 2.06                     | 0.55              |
| 50:3:1155:A:H2'   | 50:3:1156:G:O4'   | 2.07                     | 0.55              |
| 51:1:742:A:H2'    | 51:1:743:A:C8     | 2.42                     | 0.55              |
| 55:8:189:TYR:CZ   | 55:8:224:PRO:HD3  | 2.41                     | 0.55              |
| 1:b:227:VAL:HG11  | 51:1:784:G:C6     | 2.42                     | 0.55              |
| 2:c:49:GLN:CD     | 2:c:79:LEU:HD13   | 2.32                     | 0.55              |
| 14:q:66:ALA:O     | 14:q:70:GLN:HG2   | 2.06                     | 0.55              |
| 30:H:66:THR:HA    | 30:H:101:ASN:HB2  | 1.88                     | 0.55              |
| 37:O:12:ALA:HB2   | 37:O:96:VAL:HG22  | 1.88                     | 0.55              |
| 50:3:1197:A:H2'   | 50:3:1198:G:H5''  | 1.89                     | 0.55              |
| 50:3:1225:A:H5'   | 50:3:1226:C:OP2   | 2.06                     | 0.55              |
| 50:3:1346:A:H2'   | 50:3:1346:A:N3    | 2.21                     | 0.55              |
| 50:3:1516:G:H2'   | 50:3:1518:A:OP2   | 2.06                     | 0.55              |
| 55:8:115:PHE:HA   | 55:8:118:MET:HB2  | 1.89                     | 0.55              |
| 4:e:66:ILE:N      | 4:e:66:ILE:HD12   | 2.21                     | 0.55              |
| 5:f:34:ARG:NH2    | 51:1:2759:G:H1'   | 2.22                     | 0.55              |
| 8:k:13:ASN:OD1    | 8:k:97:THR:N      | 2.37                     | 0.55              |
| 15:r:68:ARG:NH1   | 15:r:90:ARG:HB2   | 2.22                     | 0.55              |
| 29:G:113:LEU:HD21 | 29:G:151:LYS:HE2  | 1.89                     | 0.55              |
| 34:L:62:GLU:C     | 34:L:66:GLU:HG2   | 2.31                     | 0.55              |
| 50:3:411:A:H1'    | 50:3:413:G:H1'    | 1.89                     | 0.55              |
| 50:3:1256:A:H1'   | 50:3:1258:G:C4    | 2.41                     | 0.55              |
| 55:8:130:LEU:CD1  | 55:8:192:LEU:HD13 | 2.36                     | 0.55              |
| 1:b:86:ARG:HG3    | 1:b:86:ARG:NH1    | 2.21                     | 0.55              |
| 3:d:23:PHE:HB2    | 3:d:114:ARG:NH2   | 2.22                     | 0.55              |
| 4:e:142:TYR:HA    | 4:e:145:VAL:CG1   | 2.36                     | 0.55              |
| 6:g:147:VAL:HG22  | 6:g:148:ALA:N     | 2.22                     | 0.55              |
| 28:F:10:LEU:HD23  | 28:F:33:HIS:CD2   | 2.40                     | 0.55              |
| 50:3:424:G:H2'    | 50:3:425:G:O4'    | 2.04                     | 0.55              |
| 50:3:429:U:H3     | 50:3:431:A:H62    | 1.53                     | 0.55              |
| 50:3:730:G:C2'    | 50:3:731:G:H5'    | 2.36                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 51:1:1311:G:H21   | 51:1:1603:A:H62  | 1.55                     | 0.55              |
| 3:d:76:PRO:HA     | 3:d:82:GLY:HA2   | 1.88                     | 0.55              |
| 5:f:2:ARG:HD3     | 5:f:5:LYS:NZ     | 2.22                     | 0.55              |
| 17:t:68:LYS:HB2   | 17:t:77:ARG:NH1  | 2.23                     | 0.55              |
| 36:N:10:ARG:HD3   | 36:N:10:ARG:N    | 2.21                     | 0.55              |
| 42:T:39:GLN:O     | 42:T:43:ALA:N    | 2.40                     | 0.55              |
| 44:V:59:GLU:HB2   | 44:V:75:VAL:HB   | 1.88                     | 0.55              |
| 47:Y:74:HIS:O     | 47:Y:78:LEU:HD23 | 2.07                     | 0.55              |
| 50:3:764:C:H2'    | 50:3:765:G:O4'   | 2.07                     | 0.55              |
| 50:3:945:G:H2'    | 50:3:945:G:N3    | 2.22                     | 0.55              |
| 50:3:1305:G:H22   | 50:3:1331:G:H2'  | 1.71                     | 0.55              |
| 51:1:968:C:H2'    | 51:1:969:G:H8    | 1.72                     | 0.55              |
| 55:8:234:ILE:HD12 | 55:8:234:ILE:N   | 2.22                     | 0.55              |
| 55:8:246:THR:OG1  | 55:8:258:GLU:HB2 | 2.07                     | 0.55              |
| 29:G:95:TRP:CZ2   | 29:G:99:MET:HB3  | 2.42                     | 0.54              |
| 40:R:16:ILE:HG12  | 50:3:1302:C:C5   | 2.42                     | 0.54              |
| 49:a:210:LYS:HD2  | 49:a:211:LYS:HB2 | 1.89                     | 0.54              |
| 50:3:1404:C:H2'   | 50:3:1405:G:C8   | 2.42                     | 0.54              |
| 51:1:558:U:H2'    | 51:1:559:G:C8    | 2.42                     | 0.54              |
| 12:o:40:ILE:HD12  | 12:o:46:GLU:O    | 2.07                     | 0.54              |
| 12:o:100:HIS:NE2  | 52:2:48:U:H4'    | 2.23                     | 0.54              |
| 29:G:45:THR:CG2   | 29:G:200:PRO:HD2 | 2.37                     | 0.54              |
| 31:I:205:LYS:HA   | 50:3:8:A:C5      | 2.43                     | 0.54              |
| 32:J:86:GLY:HA3   | 32:J:93:VAL:HG13 | 1.90                     | 0.54              |
| 33:K:14:GLN:HG3   | 33:K:17:GLN:HE21 | 1.72                     | 0.54              |
| 37:O:66:GLU:O     | 37:O:67:ILE:HG13 | 2.08                     | 0.54              |
| 46:X:31:ARG:HB2   | 46:X:56:HIS:CD2  | 2.41                     | 0.54              |
| 51:1:1112:G:H2'   | 51:1:1113:U:C6   | 2.42                     | 0.54              |
| 51:1:1723:G:H3'   | 51:1:1724:G:H8   | 1.72                     | 0.54              |
| 51:1:2086:U:H2'   | 51:1:2087:G:C8   | 2.43                     | 0.54              |
| 51:1:2196:C:O2'   | 51:1:2197:U:H5'  | 2.08                     | 0.54              |
| 51:1:2431:U:H5    | 51:1:2433:A:H62  | 1.53                     | 0.54              |
| 2:c:8:LYS:HB2     | 2:c:201:LEU:HD11 | 1.90                     | 0.54              |
| 12:o:15:ARG:HH22  | 52:2:8:C:H5''    | 1.71                     | 0.54              |
| 28:F:10:LEU:HD23  | 28:F:33:HIS:NE2  | 2.22                     | 0.54              |
| 44:V:5:ARG:HD3    | 50:3:636:U:H5''  | 1.90                     | 0.54              |
| 48:Z:16:ARG:CZ    | 48:Z:19:LYS:HD3  | 2.37                     | 0.54              |
| 50:3:701:U:H4'    | 50:3:703:G:H1'   | 1.89                     | 0.54              |
| 51:1:1231:U:H2'   | 51:1:1232:G:H8   | 1.72                     | 0.54              |
| 51:1:1422:G:H21   | 51:1:1498:C:H1'  | 1.72                     | 0.54              |
| 51:1:2183:A:H2'   | 51:1:2184:A:C8   | 2.42                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:e:79:ARG:HG3    | 4:e:80:GLN:N     | 2.21                     | 0.54              |
| 18:u:85:ARG:HH22  | 18:u:99:SER:HB2  | 1.73                     | 0.54              |
| 51:1:2329:U:H2'   | 51:1:2330:G:C8   | 2.43                     | 0.54              |
| 1:b:144:GLU:HA    | 1:b:151:GLY:HA2  | 1.89                     | 0.54              |
| 2:c:147:GLY:O     | 51:1:2052:A:H5'  | 2.08                     | 0.54              |
| 6:g:126:GLY:H     | 6:g:146:VAL:CG1  | 2.19                     | 0.54              |
| 7:j:80:HIS:CD2    | 51:1:2642:G:H5'  | 2.42                     | 0.54              |
| 9:l:29:LYS:NZ     | 51:1:566:U:H5''  | 2.21                     | 0.54              |
| 12:o:35:ILE:HD12  | 12:o:35:ILE:N    | 2.23                     | 0.54              |
| 21:x:18:SER:HB2   | 51:1:2080:A:H5'  | 1.90                     | 0.54              |
| 30:H:21:TRP:HH2   | 30:H:32:LEU:HD12 | 1.72                     | 0.54              |
| 37:O:40:ILE:HB    | 37:O:73:LEU:HB2  | 1.89                     | 0.54              |
| 50:3:31:G:N2      | 50:3:47:C:H5''   | 2.22                     | 0.54              |
| 51:1:481:G:H1'    | 51:1:506:G:N2    | 2.23                     | 0.54              |
| 51:1:1744:A:H3'   | 51:1:1745:A:H8   | 1.72                     | 0.54              |
| 53:5:44:A:H2'     | 53:5:45:G:O4'    | 2.08                     | 0.54              |
| 55:8:200:ARG:HG3  | 55:8:217:PHE:CE1 | 2.42                     | 0.54              |
| 5:f:173:ALA:HB3   | 5:f:176:LYS:OXT  | 2.08                     | 0.54              |
| 25:C:3:GLY:N      | 51:1:2283:C:O5'  | 2.40                     | 0.54              |
| 30:H:155:ARG:HH11 | 30:H:155:ARG:HG3 | 1.73                     | 0.54              |
| 32:J:44:ARG:HG2   | 32:J:72:ASN:HB2  | 1.90                     | 0.54              |
| 32:J:74:ALA:O     | 32:J:146:MET:HE3 | 2.07                     | 0.54              |
| 34:L:13:PRO:HB2   | 34:L:18:GLY:HA2  | 1.89                     | 0.54              |
| 35:M:125:ILE:HD12 | 35:M:125:ILE:N   | 2.23                     | 0.54              |
| 37:O:40:ILE:HD12  | 37:O:73:LEU:HB2  | 1.89                     | 0.54              |
| 51:1:2156:G:C2'   | 51:1:2157:G:H5'  | 2.38                     | 0.54              |
| 3:d:30:GLN:NE2    | 51:1:659:G:H21   | 2.06                     | 0.54              |
| 6:g:1:MET:N       | 6:g:21:VAL:O     | 2.41                     | 0.54              |
| 19:v:83:LYS:HE3   | 51:1:1119:U:OP1  | 2.08                     | 0.54              |
| 34:L:77:ARG:HB3   | 34:L:86:VAL:HG21 | 1.89                     | 0.54              |
| 36:N:128:LYS:HB3  | 36:N:129:ARG:HD2 | 1.90                     | 0.54              |
| 50:3:966:G:N2     | 53:5:34:C:H5'    | 2.23                     | 0.54              |
| 51:1:247:G:H4'    | 51:1:386:G:O6    | 2.08                     | 0.54              |
| 51:1:1437:C:H2'   | 51:1:1438:U:H6   | 1.72                     | 0.54              |
| 5:f:41:GLU:HA     | 5:f:54:ARG:HH21  | 1.73                     | 0.54              |
| 5:f:125:PRO:HG2   | 5:f:126:THR:H    | 1.71                     | 0.54              |
| 7:j:45:THR:HB     | 7:j:48:VAL:HG22  | 1.88                     | 0.54              |
| 30:H:192:TYR:O    | 50:3:1055:A:H2   | 1.91                     | 0.54              |
| 35:M:87:ARG:O     | 35:M:90:GLU:HG2  | 2.07                     | 0.54              |
| 43:U:67:ILE:HG22  | 43:U:71:VAL:HG23 | 1.90                     | 0.54              |
| 51:1:75:G:H22     | 51:1:111:A:H2    | 1.55                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:1:1417:C:H4'   | 51:1:1587:G:H21   | 1.73                     | 0.54              |
| 51:1:2480:C:H2'   | 51:1:2481:G:O4'   | 2.07                     | 0.54              |
| 6:g:40:THR:HG22   | 6:g:43:ASN:HB2    | 1.89                     | 0.54              |
| 43:U:18:GLN:HA    | 43:U:38:PHE:HA    | 1.90                     | 0.54              |
| 49:a:7:ARG:O      | 49:a:10:VAL:HG12  | 2.08                     | 0.54              |
| 51:1:438:G:H2'    | 51:1:439:A:C8     | 2.43                     | 0.54              |
| 51:1:2724:U:H2'   | 51:1:2725:A:C8    | 2.43                     | 0.54              |
| 51:1:2898:U:H2'   | 51:1:2899:A:H8    | 1.72                     | 0.54              |
| 52:2:48:U:H2'     | 52:2:49:C:C6      | 2.43                     | 0.54              |
| 52:2:104:A:H2'    | 52:2:105:G:O4'    | 2.07                     | 0.54              |
| 55:8:129:TYR:CE2  | 55:8:166:ILE:HG13 | 2.43                     | 0.54              |
| 4:e:32:LYS:HE2    | 4:e:91:ARG:HH11   | 1.73                     | 0.54              |
| 5:f:163:TYR:HB2   | 5:f:166:GLU:HG3   | 1.90                     | 0.54              |
| 9:l:118:THR:HG23  | 9:l:119:PRO:HD2   | 1.90                     | 0.54              |
| 12:o:79:ALA:O     | 12:o:82:ALA:HB3   | 2.08                     | 0.54              |
| 13:p:27:VAL:HG13  | 13:p:42:PHE:HB3   | 1.89                     | 0.54              |
| 51:1:1715:G:H2'   | 51:1:1716:U:H5    | 1.72                     | 0.54              |
| 1:b:266:ILE:HG21  | 1:b:269:ARG:HD2   | 1.90                     | 0.53              |
| 2:c:179:ARG:HB3   | 2:c:188:LEU:HD12  | 1.90                     | 0.53              |
| 4:e:147:ARG:HH11  | 4:e:149:ARG:HA    | 1.74                     | 0.53              |
| 5:f:156:TYR:C     | 5:f:157:LYS:HD3   | 2.33                     | 0.53              |
| 6:g:40:THR:CG2    | 6:g:43:ASN:HB2    | 2.38                     | 0.53              |
| 12:o:7:ARG:HD2    | 12:o:97:PHE:CZ    | 2.43                     | 0.53              |
| 25:C:21:THR:HG21  | 51:1:2419:U:H5''  | 1.89                     | 0.53              |
| 31:I:25:ARG:HH11  | 31:I:25:ARG:CB    | 2.17                     | 0.53              |
| 34:L:38:ALA:O     | 34:L:42:VAL:HG23  | 2.07                     | 0.53              |
| 36:N:104:THR:HG22 | 50:3:1180:A:OP1   | 2.08                     | 0.53              |
| 38:P:43:TRP:CD1   | 50:3:686:U:H4'    | 2.43                     | 0.53              |
| 44:V:25:GLU:HG3   | 44:V:40:THR:HG22  | 1.91                     | 0.53              |
| 46:X:32:THR:HG22  | 46:X:49:ALA:O     | 2.07                     | 0.53              |
| 51:1:729:G:H5'    | 51:1:730:A:H5''   | 1.90                     | 0.53              |
| 51:1:1049:C:H2'   | 51:1:1050:A:O4'   | 2.07                     | 0.53              |
| 55:8:127:ASP:HA   | 55:8:188:ALA:HB3  | 1.89                     | 0.53              |
| 1:b:32:LEU:HD13   | 1:b:102:TYR:CD2   | 2.44                     | 0.53              |
| 3:d:29:HIS:NE2    | 9:l:8:PRO:HD3     | 2.22                     | 0.53              |
| 6:g:29:PHE:CE1    | 6:g:33:GLN:HG2    | 2.43                     | 0.53              |
| 28:F:9:LYS:HE3    | 28:F:12:ARG:O     | 2.08                     | 0.53              |
| 39:Q:113:ARG:HH12 | 50:3:36:C:H4'     | 1.73                     | 0.53              |
| 44:V:74:LEU:HD23  | 44:V:75:VAL:N     | 2.23                     | 0.53              |
| 46:X:79:TYR:CE1   | 50:3:1226:C:H4'   | 2.43                     | 0.53              |
| 50:3:1527:U:O2'   | 50:3:1528:U:H5'   | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:8:197:GLY:HA3  | 55:8:323:ILE:HG13 | 1.88                     | 0.53              |
| 1:b:158:GLY:N     | 1:b:194:VAL:HG13  | 2.22                     | 0.53              |
| 2:c:100:LEU:O     | 2:c:100:LEU:HD23  | 2.07                     | 0.53              |
| 3:d:63:LYS:HD2    | 51:1:2444:G:OP2   | 2.09                     | 0.53              |
| 11:n:55:ALA:HA    | 11:n:80:PHE:CE1   | 2.44                     | 0.53              |
| 16:s:29:VAL:HG21  | 16:s:69:LEU:HD23  | 1.91                     | 0.53              |
| 18:u:89:GLY:C     | 18:u:90:LYS:HD3   | 2.34                     | 0.53              |
| 40:R:3:ILE:HG21   | 40:R:56:ARG:HG2   | 1.89                     | 0.53              |
| 42:T:23:SER:HB3   | 42:T:26:VAL:CG2   | 2.38                     | 0.53              |
| 49:a:42:VAL:HG23  | 49:a:178:VAL:HG22 | 1.90                     | 0.53              |
| 51:1:1528:A:H62   | 51:1:1543:G:H21   | 1.55                     | 0.53              |
| 55:8:33:ARG:HA    | 55:8:36:GLU:HB2   | 1.90                     | 0.53              |
| 55:8:155:TRP:NE1  | 55:8:354:ASP:OD1  | 2.42                     | 0.53              |
| 2:c:49:GLN:NE2    | 2:c:79:LEU:HD13   | 2.23                     | 0.53              |
| 3:d:143:LEU:O     | 3:d:143:LEU:HD12  | 2.08                     | 0.53              |
| 29:G:185:ILE:HG21 | 29:G:203:ASP:HB3  | 1.89                     | 0.53              |
| 30:H:113:LYS:HE2  | 30:H:184:ASN:CG   | 2.33                     | 0.53              |
| 32:J:105:ILE:CD1  | 32:J:123:LEU:HD22 | 2.37                     | 0.53              |
| 33:K:43:GLY:HA2   | 33:K:58:HIS:CE1   | 2.43                     | 0.53              |
| 42:T:76:ARG:O     | 42:T:80:LEU:HD23  | 2.08                     | 0.53              |
| 50:3:1532:U:C3'   | 50:3:1533:C:H5'   | 2.38                     | 0.53              |
| 51:1:817:C:H2'    | 51:1:818:G:O4'    | 2.08                     | 0.53              |
| 51:1:2323:G:H2'   | 51:1:2324:U:O4'   | 2.09                     | 0.53              |
| 2:c:118:PHE:CE1   | 2:c:163:GLY:HA2   | 2.43                     | 0.53              |
| 16:s:84:ARG:HB2   | 16:s:96:ILE:HG13  | 1.91                     | 0.53              |
| 18:u:43:LYS:NZ    | 18:u:45:GLN:HA    | 2.23                     | 0.53              |
| 19:v:78:GLN:HB2   | 19:v:88:HIS:HB3   | 1.90                     | 0.53              |
| 29:G:129:THR:HG23 | 29:G:132:GLU:HB3  | 1.90                     | 0.53              |
| 40:R:89:ARG:HB2   | 40:R:96:VAL:HG12  | 1.90                     | 0.53              |
| 41:S:68:ARG:HH22  | 41:S:80:ARG:HH22  | 1.56                     | 0.53              |
| 51:1:1316:U:H2'   | 51:1:1317:G:H8    | 1.72                     | 0.53              |
| 51:1:2106:U:H2'   | 51:1:2107:G:H8    | 1.71                     | 0.53              |
| 51:1:2514:U:H2'   | 51:1:2515:C:C6    | 2.43                     | 0.53              |
| 1:b:143:VAL:HG22  | 1:b:189:ALA:HB2   | 1.90                     | 0.53              |
| 3:d:8:ALA:O       | 3:d:10:SER:N      | 2.40                     | 0.53              |
| 8:k:18:ARG:CB     | 8:k:45:GLU:HB2    | 2.36                     | 0.53              |
| 14:q:107:ALA:CB   | 15:r:48:LYS:HZ2   | 2.16                     | 0.53              |
| 16:s:18:ARG:HH11  | 16:s:18:ARG:HG3   | 1.74                     | 0.53              |
| 29:G:23:ASN:H     | 29:G:189:ASN:HA   | 1.72                     | 0.53              |
| 32:J:107:GLY:CA   | 50:3:9:G:H5'      | 2.39                     | 0.53              |
| 40:R:15:VAL:HG21  | 40:R:40:GLU:OE2   | 2.08                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 51:1:968:C:H2'   | 51:1:969:G:C8     | 2.44                     | 0.53              |
| 55:8:277:ASP:OD2 | 55:8:282:LYS:HG2  | 2.09                     | 0.53              |
| 6:g:70:GLU:HG2   | 6:g:138:VAL:HG21  | 1.91                     | 0.53              |
| 12:o:63:LYS:HZ3  | 52:2:51:G:H5'     | 1.73                     | 0.53              |
| 31:I:9:LYS:CE    | 50:3:542:G:H5''   | 2.38                     | 0.53              |
| 35:M:86:LYS:HG3  | 35:M:124:ILE:HD12 | 1.90                     | 0.53              |
| 35:M:91:LEU:CD1  | 35:M:116:ARG:HG2  | 2.38                     | 0.53              |
| 37:O:59:LYS:HG3  | 50:3:973:G:OP1    | 2.08                     | 0.53              |
| 45:W:61:ALA:HB1  | 45:W:66:LEU:HB2   | 1.90                     | 0.53              |
| 46:X:77:ARG:HH12 | 50:3:1223:C:P     | 2.32                     | 0.53              |
| 49:a:7:ARG:NH1   | 49:a:218:MET:HB3  | 2.24                     | 0.53              |
| 50:3:518:C:OP2   | 50:3:530:G:H4'    | 2.08                     | 0.53              |
| 51:1:2427:C:H5'' | 51:1:2429:G:H5'   | 1.89                     | 0.53              |
| 55:8:33:ARG:HH22 | 55:8:40:GLU:CD    | 2.16                     | 0.53              |
| 4:e:120:SER:HB2  | 4:e:127:TYR:CD1   | 2.43                     | 0.53              |
| 8:k:71:ARG:HB2   | 8:k:73:ASP:OD1    | 2.08                     | 0.53              |
| 10:m:109:PRO:HG2 | 10:m:112:LEU:CB   | 2.39                     | 0.53              |
| 13:p:31:VAL:HG22 | 13:p:32:VAL:N     | 2.23                     | 0.53              |
| 18:u:17:ASP:HB3  | 18:u:20:LYS:HD2   | 1.91                     | 0.53              |
| 27:E:20:GLY:HA3  | 27:E:48:MET:HE1   | 1.90                     | 0.53              |
| 31:I:23:GLY:HA3  | 50:3:408:A:O3'    | 2.09                     | 0.53              |
| 38:P:121:ARG:HD3 | 38:P:122:PRO:O    | 2.08                     | 0.53              |
| 40:R:16:ILE:HD12 | 40:R:16:ILE:N     | 2.23                     | 0.53              |
| 40:R:79:LEU:HD13 | 40:R:86:ARG:HE    | 1.73                     | 0.53              |
| 51:1:558:U:H2'   | 51:1:559:G:H8     | 1.74                     | 0.53              |
| 51:1:2267:A:H5'' | 51:1:2268:A:H5'   | 1.91                     | 0.53              |
| 51:1:2328:A:H2'  | 51:1:2329:U:C6    | 2.44                     | 0.53              |
| 1:b:96:LYS:HE2   | 1:b:96:LYS:HA     | 1.91                     | 0.53              |
| 4:e:90:LEU:HD22  | 4:e:94:ARG:CD     | 2.39                     | 0.53              |
| 5:f:98:LYS:HB2   | 5:f:101:VAL:HG13  | 1.91                     | 0.53              |
| 8:k:64:ARG:HB2   | 8:k:83:ALA:HB3    | 1.91                     | 0.53              |
| 13:p:96:LEU:HD12 | 13:p:96:LEU:N     | 2.24                     | 0.53              |
| 23:z:11:SER:HB2  | 51:1:989:G:OP2    | 2.09                     | 0.53              |
| 44:V:26:ARG:NH2  | 50:3:237:G:H5''   | 2.23                     | 0.53              |
| 51:1:562:U:O4'   | 51:1:2036:C:H5'   | 2.08                     | 0.53              |
| 51:1:581:C:H2'   | 51:1:582:A:C8     | 2.44                     | 0.53              |
| 51:1:668:A:H2'   | 51:1:670:A:H62    | 1.72                     | 0.53              |
| 52:2:95:U:H2'    | 52:2:96:G:H8      | 1.74                     | 0.53              |
| 55:8:202:VAL:HB  | 55:8:327:VAL:HA   | 1.91                     | 0.53              |
| 1:b:124:LYS:HD3  | 1:b:125:PRO:N     | 2.25                     | 0.53              |
| 5:f:66:THR:HA    | 51:1:2747:G:O2'   | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:t:39:THR:O     | 17:t:43:ILE:HG13  | 2.08                     | 0.53              |
| 22:y:22:LEU:HD23  | 22:y:22:LEU:O     | 2.09                     | 0.53              |
| 24:B:46:GLY:HA3   | 24:B:54:ILE:CG2   | 2.39                     | 0.53              |
| 32:J:137:ARG:NE   | 50:3:1078:U:H4'   | 2.24                     | 0.53              |
| 33:K:40:GLU:OE1   | 33:K:99:ALA:HA    | 2.09                     | 0.53              |
| 33:K:79:ARG:NH1   | 50:3:671:G:H4'    | 2.24                     | 0.53              |
| 38:P:87:GLY:N     | 38:P:113:THR:HG22 | 2.20                     | 0.53              |
| 48:Z:5:VAL:HG12   | 48:Z:19:LYS:HZ2   | 1.70                     | 0.53              |
| 49:a:5:THR:HG22   | 49:a:6:LYS:N      | 2.15                     | 0.53              |
| 50:3:1296:C:H4'   | 50:3:1302:C:N4    | 2.24                     | 0.53              |
| 51:1:482:A:H1'    | 51:1:498:G:N2     | 2.24                     | 0.53              |
| 51:1:1071:G:H2'   | 51:1:1071:G:N3    | 2.24                     | 0.53              |
| 51:1:1524:G:H2'   | 51:1:1525:A:H8    | 1.74                     | 0.53              |
| 51:1:2471:A:H2'   | 51:1:2472:G:O4'   | 2.09                     | 0.53              |
| 52:2:65:U:H2'     | 52:2:66:A:H5'     | 1.91                     | 0.53              |
| 4:e:114:ARG:HG2   | 4:e:114:ARG:HH21  | 1.74                     | 0.52              |
| 5:f:24:THR:HG22   | 5:f:33:THR:CG2    | 2.37                     | 0.52              |
| 13:p:4:ILE:H      | 13:p:4:ILE:CD1    | 2.21                     | 0.52              |
| 18:u:35:VAL:HG22  | 18:u:36:GLU:H     | 1.74                     | 0.52              |
| 34:L:4:ARG:NH2    | 50:3:1345:U:H2'   | 2.23                     | 0.52              |
| 50:3:321:A:H4'    | 50:3:1436:U:H5'   | 1.91                     | 0.52              |
| 50:3:715:A:H2'    | 50:3:716:A:C8     | 2.44                     | 0.52              |
| 50:3:1128:C:O2'   | 50:3:1129:C:H5'   | 2.09                     | 0.52              |
| 55:8:117:ARG:HH21 | 55:8:361:LEU:C    | 2.17                     | 0.52              |
| 2:c:1:MET:SD      | 2:c:2:ILE:N       | 2.83                     | 0.52              |
| 6:g:57:LYS:O      | 6:g:61:VAL:HG23   | 2.08                     | 0.52              |
| 9:l:79:LEU:H      | 9:l:113:ALA:HB3   | 1.74                     | 0.52              |
| 12:o:83:LEU:HA    | 12:o:88:LYS:HZ3   | 1.75                     | 0.52              |
| 16:s:17:VAL:HG23  | 16:s:76:VAL:HG21  | 1.91                     | 0.52              |
| 27:E:38:LYS:HE3   | 51:1:2351:G:O6    | 2.09                     | 0.52              |
| 40:R:32:ILE:HG23  | 40:R:58:GLU:HG2   | 1.90                     | 0.52              |
| 45:W:53:GLN:HA    | 45:W:56:ARG:NH1   | 2.24                     | 0.52              |
| 47:Y:20:ASN:ND2   | 50:3:323:U:H5''   | 2.24                     | 0.52              |
| 50:3:92:U:H2'     | 50:3:93:U:H5'     | 1.92                     | 0.52              |
| 50:3:358:U:H2'    | 50:3:359:G:C8     | 2.44                     | 0.52              |
| 51:1:107:G:H2'    | 51:1:108:G:H8     | 1.74                     | 0.52              |
| 51:1:446:G:H4'    | 51:1:449:A:C2     | 2.44                     | 0.52              |
| 51:1:511:U:C2'    | 51:1:512:G:H5'    | 2.37                     | 0.52              |
| 51:1:1065:U:H5'   | 51:1:1066:U:OP2   | 2.09                     | 0.52              |
| 51:1:1299:G:H4'   | 51:1:1301:A:C8    | 2.44                     | 0.52              |
| 51:1:1709:U:O2'   | 51:1:2859:G:H1'   | 2.09                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:g:112:LYS:HE2  | 51:1:2220:U:OP1   | 2.10                     | 0.52              |
| 10:m:74:THR:HG21 | 10:m:86:LYS:HE3   | 1.89                     | 0.52              |
| 31:I:56:GLU:HG3  | 31:I:199:ILE:HD11 | 1.91                     | 0.52              |
| 33:K:14:GLN:O    | 33:K:18:VAL:HG13  | 2.08                     | 0.52              |
| 39:Q:47:ALA:HB1  | 50:3:520:A:OP2    | 2.09                     | 0.52              |
| 50:3:707:U:H2'   | 50:3:708:C:C6     | 2.45                     | 0.52              |
| 51:1:2527:C:H2'  | 51:1:2528:U:C6    | 2.45                     | 0.52              |
| 51:1:2563:U:C3'  | 51:1:2564:A:H5''  | 2.38                     | 0.52              |
| 1:b:181:ARG:HG3  | 1:b:181:ARG:HH11  | 1.74                     | 0.52              |
| 4:e:56:LEU:O     | 4:e:61:GLY:N      | 2.41                     | 0.52              |
| 13:p:96:LEU:HB3  | 13:p:99:LEU:HD23  | 1.91                     | 0.52              |
| 28:F:11:CYS:SG   | 28:F:14:CYS:HB2   | 2.50                     | 0.52              |
| 33:K:3:HIS:HA    | 33:K:65:GLU:HA    | 1.90                     | 0.52              |
| 33:K:68:GLN:H    | 33:K:68:GLN:CD    | 2.15                     | 0.52              |
| 40:R:21:ILE:HB   | 40:R:24:VAL:CG1   | 2.39                     | 0.52              |
| 41:S:1:ALA:HA    | 50:3:1049:U:C5    | 2.45                     | 0.52              |
| 41:S:64:ARG:NH2  | 41:S:77:GLY:HA3   | 2.24                     | 0.52              |
| 43:U:23:ASP:HB3  | 43:U:26:ASN:ND2   | 2.25                     | 0.52              |
| 47:Y:32:LYS:HE2  | 50:3:1439:G:OP1   | 2.09                     | 0.52              |
| 48:Z:23:GLU:CD   | 48:Z:24:LYS:N     | 2.67                     | 0.52              |
| 50:3:16:A:O2'    | 50:3:17:U:H5'     | 2.09                     | 0.52              |
| 50:3:189:A:H2'   | 50:3:190:A:O4'    | 2.09                     | 0.52              |
| 51:1:1458:U:H4'  | 51:1:1459:G:C8    | 2.45                     | 0.52              |
| 51:1:2283:C:H5'' | 51:1:2389:G:O2'   | 2.09                     | 0.52              |
| 51:1:2898:U:H2'  | 51:1:2899:A:C8    | 2.44                     | 0.52              |
| 55:8:17:ARG:HD2  | 55:8:20:VAL:HG21  | 1.92                     | 0.52              |
| 2:c:9:VAL:HG22   | 13:p:4:ILE:HD11   | 1.92                     | 0.52              |
| 4:e:114:ARG:HG2  | 4:e:114:ARG:NH2   | 2.24                     | 0.52              |
| 5:f:173:ALA:HB3  | 5:f:176:LYS:C     | 2.35                     | 0.52              |
| 24:B:8:THR:HG23  | 24:B:11:LYS:H     | 1.74                     | 0.52              |
| 30:H:118:SER:O   | 30:H:122:GLN:HG3  | 2.10                     | 0.52              |
| 39:Q:98:ARG:HB2  | 39:Q:116:TYR:HA   | 1.91                     | 0.52              |
| 50:3:1209:C:H4'  | 55:8:343:ARG:HH22 | 1.74                     | 0.52              |
| 51:1:1706:C:C2   | 51:1:1757:A:H5'   | 2.45                     | 0.52              |
| 51:1:2563:U:C2'  | 51:1:2564:A:H5''  | 2.38                     | 0.52              |
| 55:8:124:ASP:HB3 | 55:8:187:TYR:CE1  | 2.44                     | 0.52              |
| 6:g:72:ILE:O     | 6:g:72:ILE:HG13   | 2.09                     | 0.52              |
| 8:k:71:ARG:HD2   | 8:k:77:ILE:HD11   | 1.92                     | 0.52              |
| 17:t:1:MET:HE3   | 17:t:2:ILE:N      | 2.23                     | 0.52              |
| 34:L:72:VAL:HG23 | 34:L:140:VAL:HG22 | 1.92                     | 0.52              |
| 36:N:113:LYS:HG2 | 36:N:120:ALA:H    | 1.75                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:R:97:ARG:HG3   | 40:R:97:ARG:HH11  | 1.74                     | 0.52              |
| 43:U:14:ARG:NH1   | 50:3:618:C:H1'    | 2.24                     | 0.52              |
| 55:8:15:THR:HA    | 55:8:73:MET:HE1   | 1.91                     | 0.52              |
| 1:b:220:ARG:HG3   | 51:1:1789:A:OP1   | 2.10                     | 0.52              |
| 2:c:179:ARG:NH1   | 2:c:179:ARG:HB2   | 2.24                     | 0.52              |
| 4:e:109:ARG:HD3   | 4:e:136:ILE:CA    | 2.40                     | 0.52              |
| 5:f:116:LEU:HD21  | 5:f:120:ILE:CG2   | 2.39                     | 0.52              |
| 29:G:67:LEU:HB2   | 29:G:160:LEU:HD23 | 1.91                     | 0.52              |
| 38:P:30:ILE:HG22  | 38:P:45:THR:HA    | 1.92                     | 0.52              |
| 39:Q:23:LEU:HD22  | 39:Q:29:LYS:CE    | 2.39                     | 0.52              |
| 39:Q:115:LYS:O    | 39:Q:116:TYR:HB2  | 2.09                     | 0.52              |
| 43:U:78:VAL:O     | 43:U:78:VAL:HG22  | 2.09                     | 0.52              |
| 50:3:77:A:H2'     | 50:3:78:A:H8      | 1.75                     | 0.52              |
| 50:3:412:A:H62    | 50:3:431:A:H61    | 1.57                     | 0.52              |
| 51:1:1917:U:H2'   | 51:1:1918:A:O4'   | 2.09                     | 0.52              |
| 3:d:71:GLY:N      | 51:1:674:G:H5''   | 2.24                     | 0.52              |
| 4:e:110:ILE:HG23  | 4:e:110:ILE:O     | 2.10                     | 0.52              |
| 9:l:29:LYS:HZ3    | 51:1:566:U:H5''   | 1.73                     | 0.52              |
| 14:q:40:LYS:HD3   | 14:q:43:GLN:HE21  | 1.74                     | 0.52              |
| 29:G:37:VAL:O     | 29:G:39:ILE:HD12  | 2.10                     | 0.52              |
| 31:I:103:ARG:HH11 | 31:I:169:TRP:HH2  | 1.58                     | 0.52              |
| 37:O:6:ILE:HG13   | 37:O:76:ILE:HB    | 1.91                     | 0.52              |
| 38:P:127:ARG:HB2  | 50:3:795:C:O3'    | 2.10                     | 0.52              |
| 47:Y:67:HIS:O     | 47:Y:68:LYS:HG2   | 2.09                     | 0.52              |
| 51:1:1111:A:C2'   | 51:1:1112:G:H4'   | 2.39                     | 0.52              |
| 51:1:2105:U:H2'   | 51:1:2106:U:H5'   | 1.92                     | 0.52              |
| 51:1:2533:U:H2'   | 51:1:2534:A:O4'   | 2.09                     | 0.52              |
| 51:1:2810:A:H2'   | 51:1:2811:G:O4'   | 2.10                     | 0.52              |
| 6:g:117:LEU:HD12  | 6:g:117:LEU:N     | 2.24                     | 0.52              |
| 7:j:27:ARG:NH2    | 51:1:1142:A:H4'   | 2.25                     | 0.52              |
| 9:l:108:ALA:HB3   | 9:l:125:LEU:HG    | 1.91                     | 0.52              |
| 18:u:53:GLN:HB2   | 18:u:54:PRO:HD3   | 1.92                     | 0.52              |
| 46:X:54:ARG:HD3   | 50:3:958:A:C4     | 2.45                     | 0.52              |
| 50:3:1261:A:H5''  | 50:3:1262:C:C5    | 2.44                     | 0.52              |
| 51:1:2104:C:H42   | 51:1:2185:U:H3    | 1.57                     | 0.52              |
| 51:1:2105:U:H2'   | 51:1:2106:U:O4'   | 2.10                     | 0.52              |
| 52:2:30:C:H2'     | 52:2:31:C:H5'     | 1.91                     | 0.52              |
| 2:c:173:GLN:NE2   | 2:c:208:LYS:NZ    | 2.58                     | 0.52              |
| 32:J:12:GLU:HA    | 32:J:38:VAL:HA    | 1.92                     | 0.52              |
| 32:J:79:THR:HA    | 32:J:121:ASN:OD1  | 2.10                     | 0.52              |
| 33:K:74:LEU:HG    | 33:K:78:PHE:CE2   | 2.44                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:3:513:C:H2'    | 50:3:514:C:C6     | 2.45                     | 0.52              |
| 51:1:1063:G:H5''  | 51:1:1064:C:C6    | 2.45                     | 0.52              |
| 51:1:2358:A:H2'   | 51:1:2359:C:O4'   | 2.10                     | 0.52              |
| 51:1:2789:C:H2'   | 51:1:2893:A:N7    | 2.25                     | 0.52              |
| 9:l:54:GLN:NE2    | 51:1:2358:A:H61   | 2.07                     | 0.51              |
| 17:t:39:THR:CG2   | 17:t:42:GLU:HB2   | 2.41                     | 0.51              |
| 24:B:39:ARG:HG3   | 24:B:40:HIS:CE1   | 2.44                     | 0.51              |
| 30:H:72:PRO:HD3   | 30:H:104:GLU:HB3  | 1.92                     | 0.51              |
| 34:L:108:ARG:NH1  | 34:L:115:MET:HE2  | 2.24                     | 0.51              |
| 37:O:5:ARG:N      | 37:O:78:GLU:H     | 2.08                     | 0.51              |
| 49:a:192:LEU:O    | 49:a:192:LEU:HD23 | 2.10                     | 0.51              |
| 50:3:736:C:H2'    | 50:3:737:C:C6     | 2.45                     | 0.51              |
| 51:1:861:A:H2'    | 51:1:862:G:O4'    | 2.10                     | 0.51              |
| 51:1:1723:G:H2'   | 51:1:1724:G:H5'   | 1.91                     | 0.51              |
| 51:1:2440:C:C2'   | 51:1:2441:U:H4'   | 2.39                     | 0.51              |
| 55:8:323:ILE:HG22 | 55:8:324:ARG:HG3  | 1.91                     | 0.51              |
| 2:c:179:ARG:NH1   | 2:c:188:LEU:HD12  | 2.22                     | 0.51              |
| 3:d:122:GLU:HG2   | 3:d:123:LYS:H     | 1.75                     | 0.51              |
| 26:D:34:ARG:NH1   | 26:D:41:ARG:O     | 2.43                     | 0.51              |
| 32:J:80:LEU:HG    | 32:J:146:MET:SD   | 2.51                     | 0.51              |
| 39:Q:112:ALA:HB2  | 50:3:503:C:OP2    | 2.10                     | 0.51              |
| 48:Z:18:PHE:HD2   | 48:Z:19:LYS:HD2   | 1.76                     | 0.51              |
| 50:3:921:U:H5''   | 50:3:1082:A:H5'   | 1.90                     | 0.51              |
| 51:1:1571:A:H2'   | 51:1:1572:A:C8    | 2.46                     | 0.51              |
| 51:1:1863:G:H4'   | 51:1:2411:A:H4'   | 1.92                     | 0.51              |
| 51:1:2039:U:H2'   | 51:1:2040:G:C8    | 2.45                     | 0.51              |
| 51:1:2286:G:H4'   | 51:1:2287:A:O4'   | 2.09                     | 0.51              |
| 51:1:2329:U:H2'   | 51:1:2330:G:H8    | 1.74                     | 0.51              |
| 55:8:156:ALA:HB1  | 55:8:161:PHE:HB2  | 1.93                     | 0.51              |
| 1:b:156:SER:O     | 1:b:194:VAL:HG11  | 2.10                     | 0.51              |
| 3:d:5:LEU:HD13    | 3:d:10:SER:O      | 2.11                     | 0.51              |
| 3:d:191:ASP:O     | 3:d:195:GLN:HG3   | 2.10                     | 0.51              |
| 4:e:42:ALA:HB2    | 4:e:49:LEU:HD22   | 1.92                     | 0.51              |
| 4:e:109:ARG:HD3   | 4:e:136:ILE:O     | 2.10                     | 0.51              |
| 4:e:116:LEU:HD13  | 51:1:2304:G:H4'   | 1.92                     | 0.51              |
| 5:f:44:HIS:CG     | 5:f:45:ALA:H      | 2.29                     | 0.51              |
| 6:g:25:TYR:CG     | 51:1:2094:A:H5'   | 2.45                     | 0.51              |
| 10:m:135:VAL:O    | 10:m:135:VAL:HG13 | 2.10                     | 0.51              |
| 11:n:96:ARG:HG3   | 51:1:2882:A:H5'   | 1.92                     | 0.51              |
| 31:I:122:ILE:HG23 | 31:I:143:SER:O    | 2.10                     | 0.51              |
| 34:L:72:VAL:HG21  | 34:L:144:ALA:CB   | 2.37                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 46:X:62:THR:H    | 46:X:65:MET:CG    | 2.24                     | 0.51              |
| 50:3:570:G:H5'   | 50:3:820:U:O4'    | 2.11                     | 0.51              |
| 50:3:982:U:H4'   | 50:3:983:A:O5'    | 2.11                     | 0.51              |
| 51:1:1149:G:H2'  | 51:1:1150:C:C6    | 2.45                     | 0.51              |
| 51:1:2257:U:O2'  | 51:1:2258:C:H5'   | 2.10                     | 0.51              |
| 51:1:2591:C:H2'  | 51:1:2592:G:C8    | 2.45                     | 0.51              |
| 55:8:96:PHE:O    | 55:8:100:VAL:HG23 | 2.09                     | 0.51              |
| 1:b:75:ALA:HB1   | 1:b:93:VAL:CG2    | 2.41                     | 0.51              |
| 15:r:47:VAL:O    | 15:r:47:VAL:HG13  | 2.10                     | 0.51              |
| 23:z:46:MET:HE1  | 51:1:928:A:C2     | 2.46                     | 0.51              |
| 31:I:110:ARG:HA  | 31:I:113:ALA:HB3  | 1.92                     | 0.51              |
| 35:M:13:ILE:O    | 35:M:17:GLN:NE2   | 2.44                     | 0.51              |
| 48:Z:35:GLU:CG   | 48:Z:36:PHE:H     | 2.24                     | 0.51              |
| 50:3:722:G:H2'   | 50:3:724:G:C8     | 2.46                     | 0.51              |
| 50:3:946:A:H2'   | 50:3:947:G:H8     | 1.74                     | 0.51              |
| 51:1:255:A:H2'   | 51:1:256:A:O4'    | 2.10                     | 0.51              |
| 51:1:1817:G:N2   | 51:1:1818:U:H1'   | 2.26                     | 0.51              |
| 51:1:2078:C:H1'  | 51:1:2434:A:N3    | 2.26                     | 0.51              |
| 2:c:9:VAL:HG13   | 2:c:9:VAL:O       | 2.11                     | 0.51              |
| 6:g:31:VAL:HG23  | 6:g:32:PRO:CD     | 2.36                     | 0.51              |
| 6:g:54:LEU:O     | 6:g:57:LYS:HG2    | 2.09                     | 0.51              |
| 7:j:59:ALA:HB3   | 7:j:126:ALA:HA    | 1.93                     | 0.51              |
| 7:j:99:ARG:O     | 7:j:103:ILE:HG13  | 2.10                     | 0.51              |
| 8:k:76:VAL:HG22  | 13:p:72:VAL:HG22  | 1.91                     | 0.51              |
| 10:m:42:THR:O    | 10:m:46:ILE:HG13  | 2.11                     | 0.51              |
| 14:q:104:ALA:O   | 15:r:48:LYS:NZ    | 2.43                     | 0.51              |
| 14:q:105:PHE:O   | 14:q:109:VAL:HG23 | 2.11                     | 0.51              |
| 30:H:50:SER:HB2  | 30:H:114:LEU:HD11 | 1.93                     | 0.51              |
| 36:N:29:ILE:HG23 | 36:N:29:ILE:O     | 2.10                     | 0.51              |
| 38:P:22:ILE:HB   | 38:P:85:VAL:HA    | 1.93                     | 0.51              |
| 38:P:121:ARG:NH1 | 38:P:124:LYS:HG2  | 2.25                     | 0.51              |
| 45:W:48:ALA:HB3  | 50:3:835:U:P      | 2.50                     | 0.51              |
| 51:1:1775:U:H2'  | 51:1:1776:G:O4'   | 2.11                     | 0.51              |
| 3:d:163:ASN:ND2  | 51:1:320:A:N3     | 2.58                     | 0.51              |
| 6:g:59:ALA:O     | 6:g:62:LEU:HB3    | 2.10                     | 0.51              |
| 19:v:38:LEU:CD2  | 19:v:40:ILE:HD11  | 2.41                     | 0.51              |
| 30:H:23:ALA:HB3  | 30:H:28:PHE:HD1   | 1.74                     | 0.51              |
| 38:P:14:GLN:HG2  | 38:P:75:GLU:O     | 2.09                     | 0.51              |
| 44:V:74:LEU:HD23 | 44:V:75:VAL:C     | 2.36                     | 0.51              |
| 49:a:164:ARG:NH1 | 49:a:164:ARG:HB2  | 2.26                     | 0.51              |
| 50:3:150:U:H2'   | 50:3:151:A:C8     | 2.46                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:3:358:U:H2'    | 50:3:359:G:H8     | 1.75                     | 0.51              |
| 50:3:419:C:H2'    | 50:3:420:U:O4'    | 2.11                     | 0.51              |
| 55:8:155:TRP:CD1  | 55:8:353:LEU:HB3  | 2.45                     | 0.51              |
| 7:j:1:MET:HE1     | 15:r:13:ARG:H     | 1.75                     | 0.51              |
| 29:G:5:MET:HE2    | 29:G:5:MET:N      | 2.26                     | 0.51              |
| 31:I:164:ARG:HG3  | 31:I:164:ARG:NH1  | 2.25                     | 0.51              |
| 36:N:66:VAL:HG22  | 36:N:67:LYS:N     | 2.26                     | 0.51              |
| 36:N:115:VAL:HG13 | 37:O:62:ARG:NH1   | 2.25                     | 0.51              |
| 38:P:48:GLY:HA2   | 50:3:688:G:H5'    | 1.91                     | 0.51              |
| 40:R:51:GLN:O     | 40:R:54:THR:HG22  | 2.10                     | 0.51              |
| 43:U:47:GLU:N     | 43:U:47:GLU:OE1   | 2.44                     | 0.51              |
| 51:1:121:G:H4'    | 51:1:149:A:H5'    | 1.93                     | 0.51              |
| 51:1:281:C:N4     | 51:1:359:G:H1     | 2.08                     | 0.51              |
| 51:1:1704:C:H2'   | 51:1:1705:A:C8    | 2.46                     | 0.51              |
| 51:1:2742:G:O2'   | 51:1:2743:U:H5'   | 2.10                     | 0.51              |
| 5:f:25:ILE:O      | 5:f:26:LYS:HD3    | 2.10                     | 0.51              |
| 36:N:46:VAL:HG11  | 36:N:75:ALA:HB1   | 1.91                     | 0.51              |
| 36:N:108:ARG:O    | 50:3:1347:G:H2'   | 2.11                     | 0.51              |
| 39:Q:72:ASN:OD1   | 39:Q:73:LEU:HG    | 2.11                     | 0.51              |
| 41:S:57:SER:OG    | 50:3:1316:G:H4'   | 2.11                     | 0.51              |
| 44:V:63:CYS:HG    | 44:V:73:THR:HG1   | 1.59                     | 0.51              |
| 49:a:173:THR:HG22 | 49:a:174:THR:N    | 2.24                     | 0.51              |
| 9:l:60:ARG:HH21   | 51:1:2428:G:H21   | 1.57                     | 0.51              |
| 10:m:6:ARG:HD2    | 10:m:6:ARG:O      | 2.11                     | 0.51              |
| 25:C:36:LYS:HD3   | 25:C:45:HIS:HB3   | 1.92                     | 0.51              |
| 31:I:59:LYS:NZ    | 31:I:194:ILE:HG22 | 2.26                     | 0.51              |
| 41:S:52:ARG:HH22  | 46:X:13:HIS:CD2   | 2.29                     | 0.51              |
| 46:X:54:ARG:HD3   | 50:3:958:A:N3     | 2.25                     | 0.51              |
| 50:3:431:A:H2'    | 50:3:432:A:H8     | 1.75                     | 0.51              |
| 50:3:779:C:H2'    | 50:3:780:A:O4'    | 2.10                     | 0.51              |
| 50:3:802:A:H2'    | 50:3:803:G:O4'    | 2.10                     | 0.51              |
| 50:3:1245:C:H2'   | 50:3:1246:A:C8    | 2.46                     | 0.51              |
| 50:3:1261:A:H3'   | 50:3:1262:C:H6    | 1.74                     | 0.51              |
| 50:3:1315:U:H2'   | 50:3:1316:G:O4'   | 2.11                     | 0.51              |
| 51:1:1700:A:H2'   | 51:1:1701:A:H5'   | 1.92                     | 0.51              |
| 51:1:1802:A:H2'   | 51:1:1803:A:C8    | 2.45                     | 0.51              |
| 55:8:18:SER:CB    | 55:8:70:LEU:HD13  | 2.36                     | 0.51              |
| 2:c:4:LEU:HG      | 2:c:32:ASN:ND2    | 2.26                     | 0.51              |
| 2:c:13:ARG:HH11   | 13:p:55:HIS:HA    | 1.75                     | 0.51              |
| 3:d:30:GLN:HE22   | 51:1:659:G:H21    | 1.58                     | 0.51              |
| 3:d:97:ASN:HB2    | 3:d:100:MET:HG3   | 1.92                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:p:91:VAL:HG11 | 13:p:96:LEU:HD21  | 1.93                     | 0.51              |
| 30:H:39:ARG:HH12 | 30:H:54:ILE:HG13  | 1.76                     | 0.51              |
| 34:L:49:LEU:CD2  | 34:L:123:LEU:HD13 | 2.34                     | 0.51              |
| 39:Q:23:LEU:HD22 | 39:Q:29:LYS:HD3   | 1.93                     | 0.51              |
| 42:T:24:THR:O    | 42:T:28:VAL:HG23  | 2.09                     | 0.51              |
| 48:Z:61:ARG:HD2  | 48:Z:62:GLU:HG3   | 1.93                     | 0.51              |
| 50:3:166:U:H2'   | 50:3:167:A:C8     | 2.46                     | 0.51              |
| 50:3:742:G:H2'   | 50:3:743:A:H8     | 1.75                     | 0.51              |
| 51:1:1047:G:H2'  | 51:1:1110:G:N3    | 2.26                     | 0.51              |
| 51:1:1558:C:H5'  | 51:1:1560:G:H8    | 1.76                     | 0.51              |
| 3:d:47:LYS:O     | 3:d:83:VAL:CG2    | 2.59                     | 0.50              |
| 4:e:121:PHE:CE1  | 4:e:127:TYR:HB2   | 2.46                     | 0.50              |
| 5:f:69:ALA:HA    | 5:f:72:ASN:HB3    | 1.92                     | 0.50              |
| 15:r:70:GLU:OE1  | 15:r:70:GLU:N     | 2.43                     | 0.50              |
| 16:s:69:LEU:HG   | 16:s:107:VAL:CG2  | 2.41                     | 0.50              |
| 22:y:58:ASN:ND2  | 51:1:112:U:H5'    | 2.27                     | 0.50              |
| 27:E:1:PRO:N     | 51:1:591:U:H1'    | 2.26                     | 0.50              |
| 40:R:72:ILE:O    | 40:R:76:ILE:HG13  | 2.11                     | 0.50              |
| 50:3:50:A:H4'    | 50:3:51:A:H5'     | 1.93                     | 0.50              |
| 50:3:560:A:H5'   | 50:3:566:G:N2     | 2.26                     | 0.50              |
| 51:1:1316:U:H2'  | 51:1:1317:G:C8    | 2.46                     | 0.50              |
| 51:1:1954:G:N2   | 51:1:1956:U:H3    | 2.09                     | 0.50              |
| 51:1:2122:U:C2'  | 51:1:2123:G:H5'   | 2.42                     | 0.50              |
| 51:1:2252:G:C2   | 51:1:2253:G:H1'   | 2.45                     | 0.50              |
| 51:1:2512:C:H2'  | 51:1:2513:A:O4'   | 2.10                     | 0.50              |
| 51:1:2573:C:N4   | 55:8:257:THR:HG21 | 2.24                     | 0.50              |
| 52:2:30:C:C2'    | 52:2:31:C:H5'     | 2.41                     | 0.50              |
| 55:8:114:GLU:O   | 55:8:118:MET:HG3  | 2.11                     | 0.50              |
| 5:f:86:LEU:HB3   | 5:f:130:ILE:HG23  | 1.92                     | 0.50              |
| 6:g:5:LEU:HD12   | 6:g:17:ASP:OD1    | 2.11                     | 0.50              |
| 6:g:58:LEU:HA    | 6:g:61:VAL:CG2    | 2.41                     | 0.50              |
| 6:g:128:HIS:CG   | 6:g:129:GLU:N     | 2.79                     | 0.50              |
| 10:m:63:ILE:HG12 | 10:m:105:MET:CE   | 2.40                     | 0.50              |
| 31:I:27:ILE:HG12 | 31:I:28:ASP:N     | 2.27                     | 0.50              |
| 34:L:49:LEU:HD22 | 34:L:123:LEU:CD1  | 2.33                     | 0.50              |
| 34:L:79:VAL:HG23 | 34:L:80:GLY:N     | 2.26                     | 0.50              |
| 38:P:81:LEU:HD23 | 38:P:105:ARG:O    | 2.12                     | 0.50              |
| 48:Z:66:ARG:HD3  | 50:3:1098:C:O2'   | 2.11                     | 0.50              |
| 50:3:715:A:H2'   | 50:3:716:A:H8     | 1.74                     | 0.50              |
| 50:3:1022:A:H2'  | 50:3:1023:U:C6    | 2.46                     | 0.50              |
| 51:1:289:G:H2'   | 51:1:290:U:C6     | 2.46                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 51:1:340:A:H2'   | 51:1:341:C:O4'    | 2.10                     | 0.50              |
| 51:1:2564:A:C2   | 51:1:2647:U:H4'   | 2.47                     | 0.50              |
| 6:g:97:ARG:HH21  | 6:g:100:ALA:CB    | 2.17                     | 0.50              |
| 14:q:90:ASP:HB3  | 51:1:997:G:H5'    | 1.92                     | 0.50              |
| 30:H:42:LEU:HD23 | 30:H:54:ILE:CD1   | 2.41                     | 0.50              |
| 32:J:110:MET:HE2 | 32:J:139:THR:CG2  | 2.42                     | 0.50              |
| 34:L:94:ARG:NH2  | 50:3:938:A:O2'    | 2.44                     | 0.50              |
| 39:Q:55:ARG:HH11 | 39:Q:61:GLU:HB2   | 1.76                     | 0.50              |
| 40:R:1:ALA:O     | 40:R:3:ILE:HG23   | 2.11                     | 0.50              |
| 41:S:4:SER:HB2   | 50:3:994:A:C2     | 2.46                     | 0.50              |
| 48:Z:20:ARG:N    | 48:Z:20:ARG:HD2   | 2.26                     | 0.50              |
| 50:3:501:C:H2'   | 50:3:502:A:C8     | 2.47                     | 0.50              |
| 50:3:1477:U:H2'  | 50:3:1478:U:C6    | 2.47                     | 0.50              |
| 51:1:1454:C:C2'  | 51:1:1455:G:H5'   | 2.42                     | 0.50              |
| 51:1:1810:A:H2'  | 51:1:1811:G:O4'   | 2.11                     | 0.50              |
| 51:1:1825:U:H2'  | 51:1:1826:G:H8    | 1.77                     | 0.50              |
| 51:1:1917:U:O2'  | 51:1:1918:A:H5'   | 2.10                     | 0.50              |
| 51:1:1936:A:H2   | 51:1:1943:U:H3    | 1.58                     | 0.50              |
| 51:1:2572:A:H5'  | 51:1:2574:G:H4'   | 1.94                     | 0.50              |
| 55:8:203:ARG:HG3 | 55:8:328:LEU:HD22 | 1.93                     | 0.50              |
| 2:c:141:ARG:NH2  | 51:1:1998:A:OP2   | 2.43                     | 0.50              |
| 4:e:160:LYS:HG2  | 4:e:164:GLU:OE1   | 2.11                     | 0.50              |
| 6:g:4:ILE:N      | 6:g:37:VAL:O      | 2.42                     | 0.50              |
| 6:g:66:ASN:C     | 6:g:70:GLU:HG3    | 2.37                     | 0.50              |
| 18:u:35:VAL:HG13 | 18:u:37:GLY:H     | 1.75                     | 0.50              |
| 19:v:15:GLY:O    | 19:v:19:ARG:HG2   | 2.12                     | 0.50              |
| 25:C:24:LYS:NZ   | 25:C:31:GLU:O     | 2.44                     | 0.50              |
| 29:G:80:LYS:HA   | 29:G:90:PHE:CE2   | 2.46                     | 0.50              |
| 31:I:58:GLN:HE21 | 31:I:62:ARG:HD3   | 1.75                     | 0.50              |
| 31:I:170:LEU:C   | 31:I:170:LEU:HD12 | 2.36                     | 0.50              |
| 41:S:6:LYS:O     | 41:S:10:VAL:HG23  | 2.11                     | 0.50              |
| 44:V:19:SER:HA   | 44:V:70:LYS:HZ1   | 1.77                     | 0.50              |
| 51:1:362:A:H3'   | 51:1:363:G:C8     | 2.46                     | 0.50              |
| 51:1:742:A:H2'   | 51:1:743:A:H8     | 1.77                     | 0.50              |
| 55:8:200:ARG:HD3 | 55:8:322:GLN:CG   | 2.42                     | 0.50              |
| 2:c:122:VAL:HG11 | 2:c:141:ARG:NH2   | 2.27                     | 0.50              |
| 6:g:4:ILE:CD1    | 6:g:43:ASN:HB3    | 2.41                     | 0.50              |
| 6:g:5:LEU:HD13   | 6:g:14:SER:H      | 1.76                     | 0.50              |
| 10:m:102:LEU:N   | 10:m:102:LEU:HD12 | 2.27                     | 0.50              |
| 13:p:88:ARG:HB3  | 13:p:112:ARG:NE   | 2.26                     | 0.50              |
| 32:J:93:VAL:HG21 | 32:J:110:MET:HE1  | 1.94                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 33:K:38:ARG:HB2  | 33:K:63:ASN:HB3   | 1.94                     | 0.50              |
| 39:Q:66:ILE:HA   | 39:Q:96:THR:HG22  | 1.94                     | 0.50              |
| 48:Z:44:ARG:O    | 48:Z:48:LYS:N     | 2.37                     | 0.50              |
| 50:3:82:G:H2'    | 50:3:83:C:H5'     | 1.93                     | 0.50              |
| 50:3:501:C:H2'   | 50:3:502:A:H8     | 1.77                     | 0.50              |
| 50:3:514:C:H2'   | 50:3:515:G:H8     | 1.76                     | 0.50              |
| 51:1:1971:U:H5'  | 51:1:1972:G:H5''  | 1.93                     | 0.50              |
| 51:1:2241:A:H2'  | 51:1:2242:G:H8    | 1.77                     | 0.50              |
| 1:b:48:ILE:HG23  | 1:b:48:ILE:O      | 2.12                     | 0.50              |
| 6:g:72:ILE:HG23  | 6:g:108:VAL:HG22  | 1.93                     | 0.50              |
| 9:l:92:LEU:HD23  | 9:l:92:LEU:N      | 2.22                     | 0.50              |
| 19:v:78:GLN:HB2  | 19:v:88:HIS:O     | 2.11                     | 0.50              |
| 24:B:2:VAL:HG22  | 24:B:3:GLN:H      | 1.76                     | 0.50              |
| 33:K:5:GLU:HA    | 33:K:63:ASN:HA    | 1.93                     | 0.50              |
| 36:N:28:VAL:HG13 | 36:N:28:VAL:O     | 2.12                     | 0.50              |
| 37:O:52:LEU:HD11 | 41:S:80:ARG:HE    | 1.77                     | 0.50              |
| 39:Q:41:PRO:HB3  | 39:Q:88:ASP:HB3   | 1.92                     | 0.50              |
| 43:U:22:ALA:HA   | 43:U:33:ILE:CD1   | 2.41                     | 0.50              |
| 43:U:52:LEU:HB3  | 43:U:57:ILE:HD11  | 1.92                     | 0.50              |
| 43:U:80:LYS:N    | 43:U:80:LYS:HD2   | 2.26                     | 0.50              |
| 47:Y:66:ILE:HG23 | 47:Y:70:LYS:HD3   | 1.94                     | 0.50              |
| 50:3:1330:U:H2'  | 50:3:1331:G:O4'   | 2.11                     | 0.50              |
| 51:1:738:G:O2'   | 51:1:739:A:H5'    | 2.12                     | 0.50              |
| 51:1:796:C:H2'   | 51:1:797:G:C8     | 2.46                     | 0.50              |
| 51:1:948:C:H2'   | 51:1:949:G:H8     | 1.76                     | 0.50              |
| 51:1:1268:A:H2'  | 51:1:1269:A:O4'   | 2.12                     | 0.50              |
| 53:5:29:G:H2'    | 53:5:30:G:H8      | 1.76                     | 0.50              |
| 55:8:22:ARG:NH2  | 55:8:70:LEU:HB2   | 2.26                     | 0.50              |
| 55:8:194:THR:HB  | 55:8:361:LEU:HD12 | 1.93                     | 0.50              |
| 55:8:340:VAL:O   | 55:8:340:VAL:HG13 | 2.12                     | 0.50              |
| 12:o:5:SER:O     | 12:o:9:ARG:N      | 2.39                     | 0.50              |
| 25:C:9:LYS:HE3   | 25:C:19:PHE:CG    | 2.46                     | 0.50              |
| 30:H:107:LYS:HG3 | 30:H:110:LEU:H    | 1.77                     | 0.50              |
| 38:P:23:HIS:CD2  | 50:3:706:A:H5''   | 2.47                     | 0.50              |
| 39:Q:119:LYS:HA  | 50:3:36:C:H5''    | 1.94                     | 0.50              |
| 49:a:16:ASP:HB2  | 49:a:19:LYS:CG    | 2.42                     | 0.50              |
| 50:3:560:A:H4'   | 50:3:561:U:H5'    | 1.92                     | 0.50              |
| 51:1:2029:G:O6   | 51:1:2032:G:H5''  | 2.12                     | 0.50              |
| 52:2:3:C:H3'     | 52:2:4:C:C5'      | 2.40                     | 0.50              |
| 3:d:3:LEU:HD11   | 3:d:14:VAL:CG1    | 2.41                     | 0.50              |
| 10:m:35:ALA:CB   | 10:m:102:LEU:HD11 | 2.39                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 16:s:20:VAL:HG21  | 16:s:43:ALA:HB3  | 1.93                     | 0.50              |
| 24:B:24:VAL:O     | 24:B:25:THR:HG22 | 2.12                     | 0.50              |
| 29:G:160:LEU:HD12 | 29:G:175:ALA:HB2 | 1.94                     | 0.50              |
| 31:I:184:LYS:O    | 31:I:184:LYS:HD2 | 2.12                     | 0.50              |
| 35:M:46:GLU:HB2   | 35:M:61:THR:CG2  | 2.42                     | 0.50              |
| 38:P:127:ARG:HH22 | 50:3:1522:U:H5'' | 1.77                     | 0.50              |
| 49:a:218:MET:HG2  | 51:1:2174:C:H1'  | 1.93                     | 0.50              |
| 50:3:434:U:H2'    | 50:3:435:A:C8    | 2.46                     | 0.50              |
| 51:1:528:A:N1     | 51:1:2042:A:H2'  | 2.27                     | 0.50              |
| 51:1:2215:C:H2'   | 51:1:2216:G:C8   | 2.47                     | 0.50              |
| 51:1:2249:U:H3'   | 51:1:2250:G:H5'  | 1.93                     | 0.50              |
| 51:1:2591:C:H2'   | 51:1:2592:G:H8   | 1.77                     | 0.50              |
| 1:b:213:ARG:NH1   | 51:1:1566:A:H5'  | 2.27                     | 0.50              |
| 4:e:35:LEU:HD12   | 4:e:88:VAL:CG1   | 2.42                     | 0.50              |
| 4:e:172:PHE:O     | 4:e:173:ASP:HB2  | 2.12                     | 0.50              |
| 17:t:25:GLU:OE2   | 17:t:26:LYS:HB2  | 2.12                     | 0.50              |
| 17:t:51:PHE:O     | 17:t:52:GLU:HG2  | 2.11                     | 0.50              |
| 23:z:5:LYS:HB2    | 23:z:57:GLU:HB2  | 1.94                     | 0.50              |
| 26:D:33:ARG:O     | 26:D:36:ALA:HB3  | 2.12                     | 0.50              |
| 31:I:197:HIS:O    | 31:I:201:GLU:HG3 | 2.11                     | 0.50              |
| 33:K:3:HIS:CE1    | 33:K:65:GLU:HB2  | 2.47                     | 0.50              |
| 39:Q:77:SER:HB2   | 39:Q:102:ASP:HB3 | 1.94                     | 0.50              |
| 51:1:279:A:C2'    | 51:1:280:U:H5'   | 2.42                     | 0.50              |
| 51:1:467:G:O2'    | 51:1:468:G:H5'   | 2.12                     | 0.50              |
| 51:1:1357:C:H2'   | 51:1:1358:G:O4'  | 2.12                     | 0.50              |
| 51:1:1538:G:O2'   | 51:1:1539:U:H5'  | 2.12                     | 0.50              |
| 51:1:2861:U:H2'   | 51:1:2862:G:H8   | 1.76                     | 0.50              |
| 3:d:55:SER:OG     | 51:1:468:G:H5''  | 2.12                     | 0.49              |
| 3:d:88:ARG:HB3    | 3:d:89:PRO:HD2   | 1.93                     | 0.49              |
| 26:D:29:GLN:O     | 26:D:33:ARG:HG3  | 2.12                     | 0.49              |
| 34:L:84:TYR:N     | 34:L:84:TYR:CD1  | 2.79                     | 0.49              |
| 35:M:91:LEU:HD13  | 35:M:116:ARG:HG2 | 1.94                     | 0.49              |
| 37:O:65:TYR:OH    | 41:S:84:ARG:HG3  | 2.12                     | 0.49              |
| 38:P:123:PRO:O    | 38:P:124:LYS:HE2 | 2.11                     | 0.49              |
| 46:X:5:LYS:HG2    | 50:3:1313:U:P    | 2.51                     | 0.49              |
| 46:X:60:PHE:CD2   | 46:X:62:THR:HG22 | 2.47                     | 0.49              |
| 50:3:1497:G:C2'   | 50:3:1498:U:H5'  | 2.42                     | 0.49              |
| 51:1:176:A:O2'    | 51:1:177:G:H5'   | 2.12                     | 0.49              |
| 51:1:1427:A:H4'   | 51:1:1428:C:C5'  | 2.42                     | 0.49              |
| 51:1:1713:A:H1'   | 51:1:1715:G:O2'  | 2.11                     | 0.49              |
| 55:8:25:LEU:HD21  | 55:8:66:VAL:HG21 | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:d:145:ASP:HA    | 3:d:166:LYS:HB3   | 1.93                     | 0.49              |
| 4:e:65:LEU:HD22   | 52:2:42:C:C5      | 2.47                     | 0.49              |
| 9:l:93:ASN:C      | 9:l:95:LEU:H      | 2.19                     | 0.49              |
| 14:q:48:ASP:HA    | 14:q:51:GLN:HB2   | 1.93                     | 0.49              |
| 16:s:28:LYS:HG2   | 16:s:70:LYS:HE3   | 1.93                     | 0.49              |
| 20:w:28:LEU:HD12  | 51:1:2354:C:OP1   | 2.12                     | 0.49              |
| 29:G:115:ASP:HA   | 29:G:118:THR:HG22 | 1.92                     | 0.49              |
| 50:3:912:C:O2'    | 50:3:913:A:H5'    | 2.11                     | 0.49              |
| 51:1:492:A:H2'    | 51:1:493:G:O4'    | 2.12                     | 0.49              |
| 51:1:1429:G:H2'   | 51:1:1430:G:H8    | 1.77                     | 0.49              |
| 1:b:78:GLU:N      | 1:b:92:LEU:O      | 2.41                     | 0.49              |
| 7:j:35:ARG:HG2    | 7:j:40:HIS:CD2    | 2.48                     | 0.49              |
| 7:j:56:VAL:C      | 7:j:57:LEU:HD12   | 2.36                     | 0.49              |
| 12:o:25:ARG:NH1   | 12:o:40:ILE:HG21  | 2.26                     | 0.49              |
| 14:q:5:ARG:HG3    | 51:1:584:C:OP2    | 2.12                     | 0.49              |
| 18:u:35:VAL:HG22  | 18:u:36:GLU:N     | 2.27                     | 0.49              |
| 21:x:7:THR:OG1    | 21:x:9:LYS:HG3    | 2.12                     | 0.49              |
| 29:G:132:GLU:OE2  | 29:G:135:MET:HE3  | 2.12                     | 0.49              |
| 36:N:118:ARG:HB2  | 36:N:122:ARG:HD2  | 1.94                     | 0.49              |
| 42:T:79:GLN:NE2   | 42:T:83:ARG:HB2   | 2.27                     | 0.49              |
| 47:Y:2:ASN:HD22   | 47:Y:4:LYS:HZ3    | 1.60                     | 0.49              |
| 48:Z:5:VAL:HB     | 48:Z:18:PHE:CE2   | 2.47                     | 0.49              |
| 50:3:493:A:H2'    | 50:3:494:G:N7     | 2.27                     | 0.49              |
| 50:3:1060:U:H2'   | 50:3:1061:G:C8    | 2.48                     | 0.49              |
| 51:1:280:U:H2'    | 51:1:281:C:C6     | 2.47                     | 0.49              |
| 51:1:767:U:H2'    | 51:1:768:G:H8     | 1.77                     | 0.49              |
| 51:1:827:U:H4'    | 51:1:828:U:C5     | 2.47                     | 0.49              |
| 51:1:1086:A:H3'   | 51:1:1086:A:N3    | 2.28                     | 0.49              |
| 51:1:2861:U:H2'   | 51:1:2862:G:C8    | 2.48                     | 0.49              |
| 55:8:63:LEU:HD12  | 55:8:64:GLU:HG2   | 1.94                     | 0.49              |
| 4:e:2:LYS:HA      | 4:e:5:ASP:OD2     | 2.12                     | 0.49              |
| 4:e:68:LYS:HA     | 4:e:82:TYR:O      | 2.13                     | 0.49              |
| 5:f:106:LEU:N     | 5:f:106:LEU:HD23  | 2.27                     | 0.49              |
| 24:B:3:GLN:HA     | 51:1:2615:U:C2    | 2.47                     | 0.49              |
| 29:G:162:VAL:HG12 | 29:G:163:ILE:N    | 2.26                     | 0.49              |
| 30:H:12:GLY:HA3   | 41:S:96:LYS:HD3   | 1.94                     | 0.49              |
| 31:I:131:ILE:H    | 31:I:131:ILE:CD1  | 2.23                     | 0.49              |
| 35:M:49:LYS:HB3   | 35:M:51:GLU:HG3   | 1.94                     | 0.49              |
| 36:N:117:LEU:HG   | 36:N:123:ARG:HD3  | 1.94                     | 0.49              |
| 48:Z:39:LYS:HB2   | 48:Z:40:PRO:CD    | 2.43                     | 0.49              |
| 51:1:1190:G:H2'   | 51:1:1191:G:H8    | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:1:2710:C:H2'   | 51:1:2711:A:C8    | 2.48                     | 0.49              |
| 52:2:51:G:O2'     | 52:2:52:A:H5'     | 2.11                     | 0.49              |
| 55:8:198:VAL:HB   | 55:8:321:SER:HB3  | 1.93                     | 0.49              |
| 3:d:130:LYS:HA    | 51:1:321:U:OP2    | 2.13                     | 0.49              |
| 10:m:23:GLY:O     | 10:m:101:VAL:HG22 | 2.12                     | 0.49              |
| 12:o:67:ASN:HA    | 52:2:50:A:OP2     | 2.12                     | 0.49              |
| 17:t:62:VAL:HG21  | 51:1:1601:G:OP1   | 2.12                     | 0.49              |
| 30:H:4:VAL:HG23   | 30:H:5:HIS:N      | 2.22                     | 0.49              |
| 50:3:1299:A:H2'   | 50:3:1300:G:H4'   | 1.95                     | 0.49              |
| 51:1:184:C:H2'    | 51:1:185:G:C8     | 2.48                     | 0.49              |
| 51:1:857:G:H2'    | 51:1:858:G:O4'    | 2.12                     | 0.49              |
| 51:1:974:G:N3     | 51:1:974:G:H2'    | 2.28                     | 0.49              |
| 55:8:17:ARG:NH2   | 55:8:362:LYS:HD3  | 2.22                     | 0.49              |
| 55:8:110:LEU:O    | 55:8:110:LEU:HD23 | 2.12                     | 0.49              |
| 2:c:102:ALA:HA    | 2:c:180:VAL:HG21  | 1.95                     | 0.49              |
| 7:j:129:GLU:OE2   | 7:j:130:HIS:O     | 2.31                     | 0.49              |
| 28:F:25:VAL:HB    | 28:F:35:GLN:HG3   | 1.95                     | 0.49              |
| 29:G:23:ASN:N     | 29:G:189:ASN:HA   | 2.28                     | 0.49              |
| 35:M:24:VAL:HB    | 35:M:60:LEU:HD12  | 1.93                     | 0.49              |
| 42:T:27:GLN:O     | 42:T:31:LEU:HD13  | 2.12                     | 0.49              |
| 49:a:185:LEU:HD23 | 49:a:185:LEU:C    | 2.38                     | 0.49              |
| 51:1:717:C:H2'    | 51:1:718:A:H5'    | 1.95                     | 0.49              |
| 55:8:10:ARG:HH22  | 55:8:110:LEU:HD13 | 1.77                     | 0.49              |
| 1:b:124:LYS:H     | 1:b:191:LEU:HD12  | 1.77                     | 0.49              |
| 3:d:46:GLN:HE22   | 3:d:87:ALA:HB3    | 1.78                     | 0.49              |
| 5:f:90:GLY:HA3    | 5:f:93:TYR:CE2    | 2.48                     | 0.49              |
| 11:n:35:LYS:HB2   | 11:n:112:TYR:CE1  | 2.48                     | 0.49              |
| 16:s:9:HIS:CE1    | 16:s:100:THR:HG21 | 2.48                     | 0.49              |
| 30:H:55:VAL:CG2   | 30:H:66:THR:HB    | 2.43                     | 0.49              |
| 32:J:10:LEU:HD23  | 32:J:10:LEU:N     | 2.22                     | 0.49              |
| 36:N:105:ARG:HH11 | 36:N:105:ARG:HG3  | 1.77                     | 0.49              |
| 37:O:23:ALA:O     | 37:O:27:GLU:HG2   | 2.12                     | 0.49              |
| 39:Q:49:ARG:HH22  | 50:3:522:C:H41    | 1.60                     | 0.49              |
| 40:R:76:ILE:O     | 40:R:80:MET:HG2   | 2.13                     | 0.49              |
| 41:S:84:ARG:O     | 41:S:88:MET:HG2   | 2.11                     | 0.49              |
| 43:U:53:ASP:O     | 43:U:57:ILE:HG13  | 2.12                     | 0.49              |
| 50:3:321:A:H2'    | 50:3:322:C:C6     | 2.47                     | 0.49              |
| 50:3:818:G:H3'    | 50:3:819:A:H5'    | 1.94                     | 0.49              |
| 50:3:1211:U:H4'   | 50:3:1213:A:C4    | 2.48                     | 0.49              |
| 51:1:1258:U:H2'   | 51:1:1259:G:C8    | 2.48                     | 0.49              |
| 51:1:1370:C:H2'   | 51:1:1371:G:O4'   | 2.13                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 51:1:1478:G:N2    | 51:1:1560:G:H1'  | 2.28                     | 0.49              |
| 51:1:1609:A:H1'   | 51:1:1616:A:C1'  | 2.43                     | 0.49              |
| 51:1:2178:C:H2'   | 51:1:2179:C:O4'  | 2.13                     | 0.49              |
| 55:8:173:VAL:HG23 | 55:8:174:ALA:N   | 2.27                     | 0.49              |
| 4:e:73:VAL:HG22   | 4:e:74:ALA:N     | 2.28                     | 0.49              |
| 4:e:167:ALA:O     | 4:e:170:ALA:HB3  | 2.13                     | 0.49              |
| 10:m:109:PRO:HG2  | 10:m:112:LEU:HB2 | 1.95                     | 0.49              |
| 13:p:28:LYS:HB3   | 13:p:39:LEU:HD11 | 1.94                     | 0.49              |
| 21:x:67:LEU:O     | 21:x:71:ARG:HG3  | 2.11                     | 0.49              |
| 30:H:21:TRP:CH2   | 30:H:32:LEU:HD12 | 2.47                     | 0.49              |
| 34:L:67:ASN:O     | 34:L:137:ARG:NH1 | 2.45                     | 0.49              |
| 48:Z:23:GLU:C     | 48:Z:25:ALA:H    | 2.20                     | 0.49              |
| 48:Z:23:GLU:OE1   | 48:Z:27:VAL:HG12 | 2.13                     | 0.49              |
| 51:1:967:U:H2'    | 51:1:968:C:C6    | 2.48                     | 0.49              |
| 51:1:1786:A:H1'   | 51:1:1938:A:N6   | 2.27                     | 0.49              |
| 51:1:1796:U:H2'   | 51:1:1797:G:H8   | 1.78                     | 0.49              |
| 52:2:12:C:H2'     | 52:2:13:G:H4'    | 1.95                     | 0.49              |
| 55:8:37:VAL:O     | 55:8:41:LEU:HD23 | 2.13                     | 0.49              |
| 55:8:152:TYR:OH   | 55:8:199:HIS:NE2 | 2.39                     | 0.49              |
| 55:8:245:ARG:HA   | 55:8:259:SER:HA  | 1.94                     | 0.49              |
| 1:b:229:HIS:CD2   | 1:b:246:PRO:HG3  | 2.48                     | 0.49              |
| 2:c:40:LEU:H      | 2:c:40:LEU:CD1   | 2.25                     | 0.49              |
| 2:c:186:LEU:HD21  | 13:p:3:ILE:HG21  | 1.94                     | 0.49              |
| 5:f:174:LYS:HD2   | 51:1:2530:A:H5'  | 1.94                     | 0.49              |
| 6:g:134:VAL:CG2   | 6:g:138:VAL:HG13 | 2.41                     | 0.49              |
| 10:m:73:ILE:HG12  | 10:m:93:VAL:HG22 | 1.95                     | 0.49              |
| 13:p:105:LYS:HG2  | 50:3:1432:G:OP2  | 2.11                     | 0.49              |
| 14:q:90:ASP:OD2   | 15:r:11:GLN:HG2  | 2.12                     | 0.49              |
| 17:t:32:LEU:N     | 17:t:32:LEU:HD23 | 2.28                     | 0.49              |
| 27:E:31:ILE:HD11  | 27:E:34:LYS:HG2  | 1.95                     | 0.49              |
| 30:H:130:ARG:HD3  | 30:H:130:ARG:N   | 2.28                     | 0.49              |
| 34:L:90:VAL:CG1   | 34:L:95:ARG:HG2  | 2.30                     | 0.49              |
| 37:O:40:ILE:HD12  | 37:O:73:LEU:HB3  | 1.93                     | 0.49              |
| 37:O:58:ASN:HB3   | 37:O:61:ALA:HB3  | 1.94                     | 0.49              |
| 43:U:36:VAL:HG23  | 43:U:53:ASP:HB3  | 1.94                     | 0.49              |
| 43:U:52:LEU:HD12  | 43:U:52:LEU:N    | 2.28                     | 0.49              |
| 44:V:74:LEU:HD23  | 44:V:74:LEU:C    | 2.38                     | 0.49              |
| 50:3:858:G:O6     | 50:3:869:G:H3'   | 2.13                     | 0.49              |
| 51:1:704:G:H1'    | 51:1:727:A:H61   | 1.77                     | 0.49              |
| 51:1:1140:C:H2'   | 51:1:1141:U:H5'  | 1.95                     | 0.49              |
| 51:1:1278:C:H2'   | 51:1:1279:G:H8   | 1.78                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 51:1:1409:U:H2'  | 51:1:1410:G:H8   | 1.77                     | 0.49              |
| 51:1:1416:G:N2   | 51:1:1585:C:H41  | 2.11                     | 0.49              |
| 51:1:1718:G:H1   | 51:1:1742:U:H3   | 1.61                     | 0.49              |
| 51:1:2291:U:O2'  | 51:1:2374:C:H1'  | 2.12                     | 0.49              |
| 51:1:2655:G:HO2' | 51:1:2656:U:H5   | 1.61                     | 0.49              |
| 51:1:2716:C:O2'  | 51:1:2717:C:H5'  | 2.13                     | 0.49              |
| 52:2:39:A:H1'    | 52:2:47:C:O2     | 2.13                     | 0.49              |
| 4:e:36:ASN:OD1   | 51:1:2313:C:H4'  | 2.13                     | 0.49              |
| 6:g:25:TYR:N     | 51:1:2093:G:H4'  | 2.28                     | 0.49              |
| 8:k:58:LEU:N     | 8:k:58:LEU:HD23  | 2.27                     | 0.49              |
| 8:k:99:ILE:HD13  | 8:k:115:ILE:HG23 | 1.94                     | 0.49              |
| 10:m:47:GLU:OE2  | 10:m:51:ARG:HB2  | 2.13                     | 0.49              |
| 11:n:53:THR:OG1  | 51:1:2840:C:H5'' | 2.13                     | 0.49              |
| 23:z:45:GLY:HA3  | 51:1:852:U:H5'   | 1.94                     | 0.49              |
| 31:I:85:THR:HA   | 31:I:88:ASN:ND2  | 2.25                     | 0.49              |
| 33:K:35:LYS:C    | 33:K:64:VAL:HG23 | 2.38                     | 0.49              |
| 35:M:113:ARG:O   | 35:M:117:GLN:HG3 | 2.12                     | 0.49              |
| 37:O:15:HIS:CE1  | 37:O:16:ARG:HG3  | 2.48                     | 0.49              |
| 51:1:2343:U:H2'  | 51:1:2344:U:C6   | 2.48                     | 0.49              |
| 55:8:124:ASP:O   | 55:8:187:TYR:HA  | 2.13                     | 0.49              |
| 1:b:119:VAL:HG23 | 1:b:120:ASP:OD1  | 2.12                     | 0.48              |
| 5:f:106:LEU:HD23 | 5:f:106:LEU:H    | 1.78                     | 0.48              |
| 13:p:82:SER:C    | 13:p:83:ILE:HD12 | 2.38                     | 0.48              |
| 19:v:60:VAL:HG22 | 19:v:73:LYS:HE2  | 1.95                     | 0.48              |
| 21:x:56:ARG:NH2  | 51:1:400:G:N7    | 2.61                     | 0.48              |
| 23:z:13:ILE:HD12 | 51:1:988:A:C8    | 2.48                     | 0.48              |
| 27:E:1:PRO:H3    | 51:1:591:U:H1'   | 1.77                     | 0.48              |
| 29:G:125:PHE:HD1 | 29:G:133:ALA:HB1 | 1.76                     | 0.48              |
| 31:I:176:LYS:O   | 31:I:177:MET:HB2 | 2.12                     | 0.48              |
| 33:K:100:SER:N   | 33:K:101:PRO:HD2 | 2.28                     | 0.48              |
| 50:3:130:A:O2'   | 50:3:264:C:H5'   | 2.12                     | 0.48              |
| 50:3:742:G:H2'   | 50:3:743:A:C8    | 2.48                     | 0.48              |
| 50:3:1003:G:H21  | 50:3:1005:A:H5'  | 1.77                     | 0.48              |
| 51:1:357:C:H2'   | 51:1:358:U:C6    | 2.48                     | 0.48              |
| 51:1:1239:G:H2'  | 51:1:1240:U:O4'  | 2.12                     | 0.48              |
| 51:1:1298:C:H2'  | 51:1:1299:G:O4'  | 2.13                     | 0.48              |
| 51:1:1479:G:H4'  | 51:1:1560:G:H21  | 1.77                     | 0.48              |
| 51:1:2055:C:H5'  | 51:1:2056:G:O5'  | 2.12                     | 0.48              |
| 51:1:2308:G:H3'  | 51:1:2309:A:C5'  | 2.43                     | 0.48              |
| 51:1:2636:C:H2'  | 51:1:2637:U:C6   | 2.48                     | 0.48              |
| 1:b:64:VAL:HG13  | 1:b:66:PHE:CD1   | 2.47                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:148:GLY:O    | 51:1:2205:A:H5'  | 2.14                     | 0.48              |
| 6:g:40:THR:HG22  | 6:g:43:ASN:HD22  | 1.76                     | 0.48              |
| 9:l:92:LEU:H     | 9:l:92:LEU:CD2   | 2.21                     | 0.48              |
| 12:o:87:ILE:C    | 12:o:88:LYS:HD3  | 2.38                     | 0.48              |
| 30:H:70:ALA:HB1  | 30:H:108:PRO:HG3 | 1.94                     | 0.48              |
| 31:I:184:LYS:HD2 | 31:I:184:LYS:C   | 2.38                     | 0.48              |
| 32:J:149:PRO:HA  | 35:M:98:LEU:HD11 | 1.94                     | 0.48              |
| 35:M:3:GLN:HB2   | 50:3:587:G:C4'   | 2.43                     | 0.48              |
| 39:Q:27:PRO:O    | 39:Q:28:GLN:HG3  | 2.13                     | 0.48              |
| 46:X:35:ARG:O    | 46:X:71:GLY:N    | 2.47                     | 0.48              |
| 47:Y:80:ALA:O    | 47:Y:84:LYS:HG3  | 2.14                     | 0.48              |
| 50:3:731:G:O2'   | 50:3:732:C:H5'   | 2.12                     | 0.48              |
| 51:1:875:G:O2'   | 51:1:876:C:H5'   | 2.12                     | 0.48              |
| 51:1:2599:G:H2'  | 51:1:2600:A:C8   | 2.47                     | 0.48              |
| 55:8:70:LEU:HA   | 55:8:73:MET:HB3  | 1.95                     | 0.48              |
| 1:b:155:ARG:HD3  | 51:1:1818:U:C5   | 2.48                     | 0.48              |
| 7:j:101:ILE:H    | 7:j:101:ILE:CD1  | 2.25                     | 0.48              |
| 35:M:14:ARG:CG   | 35:M:74:ILE:HG22 | 2.39                     | 0.48              |
| 40:R:24:VAL:HG23 | 40:R:28:ARG:HB3  | 1.94                     | 0.48              |
| 40:R:67:ASP:O    | 40:R:71:GLU:N    | 2.42                     | 0.48              |
| 47:Y:27:MET:O    | 47:Y:31:ILE:HG13 | 2.12                     | 0.48              |
| 50:3:328:C:H5'   | 50:3:329:A:H5'   | 1.95                     | 0.48              |
| 1:b:224:MET:HB3  | 1:b:228:ASP:HB2  | 1.95                     | 0.48              |
| 5:f:103:ASN:C    | 5:f:104:LEU:HD22 | 2.38                     | 0.48              |
| 6:g:140:ALA:O    | 6:g:142:VAL:HG23 | 2.12                     | 0.48              |
| 7:j:113:PRO:HD2  | 51:1:558:U:P     | 2.53                     | 0.48              |
| 9:l:126:ARG:HH21 | 9:l:126:ARG:HG2  | 1.77                     | 0.48              |
| 10:m:3:GLN:HE21  | 10:m:92:TRP:NE1  | 2.06                     | 0.48              |
| 20:w:36:GLN:NE2  | 20:w:39:THR:HA   | 2.27                     | 0.48              |
| 31:I:80:ARG:HG2  | 31:I:80:ARG:NH1  | 2.29                     | 0.48              |
| 33:K:5:GLU:CD    | 33:K:5:GLU:N     | 2.71                     | 0.48              |
| 34:L:43:TYR:O    | 34:L:47:GLU:HG3  | 2.14                     | 0.48              |
| 34:L:84:TYR:CE2  | 34:L:86:VAL:HG22 | 2.47                     | 0.48              |
| 35:M:126:CYS:SG  | 35:M:127:TYR:N   | 2.86                     | 0.48              |
| 39:Q:32:VAL:HG23 | 39:Q:34:THR:HG23 | 1.95                     | 0.48              |
| 42:T:79:GLN:NE2  | 42:T:82:GLU:OE2  | 2.47                     | 0.48              |
| 49:a:181:ASP:HB3 | 49:a:184:LYS:HB2 | 1.95                     | 0.48              |
| 50:3:150:U:H3    | 50:3:171:A:H62   | 1.62                     | 0.48              |
| 51:1:8:C:H2'     | 51:1:9:G:O4'     | 2.13                     | 0.48              |
| 51:1:851:C:H2'   | 51:1:852:U:C6    | 2.48                     | 0.48              |
| 51:1:1846:G:C2'  | 51:1:1847:A:H4'  | 2.43                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 51:1:2082:A:H2'   | 51:1:2083:G:O4'  | 2.13                     | 0.48              |
| 51:1:2308:G:H5'   | 51:1:2309:A:OP2  | 2.14                     | 0.48              |
| 52:2:51:G:H2'     | 52:2:52:A:O4'    | 2.13                     | 0.48              |
| 55:8:254:VAL:HG22 | 55:8:255:ASN:N   | 2.28                     | 0.48              |
| 5:f:85:LYS:HE3    | 5:f:164:ALA:O    | 2.14                     | 0.48              |
| 32:J:64:GLU:C     | 32:J:68:ARG:NH1  | 2.72                     | 0.48              |
| 32:J:107:GLY:HA3  | 50:3:9:G:H5'     | 1.95                     | 0.48              |
| 37:O:80:THR:O     | 37:O:84:VAL:HG23 | 2.14                     | 0.48              |
| 38:P:27:ASN:HB3   | 38:P:56:LYS:NZ   | 2.27                     | 0.48              |
| 38:P:85:VAL:CG1   | 38:P:111:ASP:HA  | 2.43                     | 0.48              |
| 39:Q:23:LEU:HD22  | 39:Q:29:LYS:HZ2  | 1.75                     | 0.48              |
| 42:T:45:HIS:O     | 42:T:47:LYS:N    | 2.47                     | 0.48              |
| 50:3:631:C:H3'    | 50:3:632:U:H5'   | 1.95                     | 0.48              |
| 51:1:64:A:H2'     | 51:1:65:U:C6     | 2.48                     | 0.48              |
| 51:1:176:A:H3'    | 51:1:177:G:N2    | 2.28                     | 0.48              |
| 51:1:466:A:C2'    | 51:1:467:G:H5'   | 2.43                     | 0.48              |
| 51:1:1060:U:C4'   | 51:1:1062:G:H5'' | 2.43                     | 0.48              |
| 51:1:1093:G:H3'   | 51:1:1094:U:C5'  | 2.44                     | 0.48              |
| 52:2:95:U:H2'     | 52:2:96:G:C8     | 2.49                     | 0.48              |
| 53:5:43:A:H2'     | 53:5:44:A:C8     | 2.49                     | 0.48              |
| 5:f:69:ALA:HB3    | 51:1:2747:G:H5'' | 1.96                     | 0.48              |
| 6:g:66:ASN:O      | 6:g:70:GLU:N     | 2.46                     | 0.48              |
| 15:r:96:VAL:HG22  | 15:r:97:LYS:N    | 2.28                     | 0.48              |
| 18:u:94:PHE:HD2   | 18:u:99:SER:HA   | 1.78                     | 0.48              |
| 21:x:16:ASN:HB2   | 21:x:24:THR:CG2  | 2.44                     | 0.48              |
| 22:y:2:LYS:O      | 22:y:6:LEU:HB2   | 2.14                     | 0.48              |
| 22:y:48:ARG:HG3   | 22:y:48:ARG:HH11 | 1.77                     | 0.48              |
| 26:D:11:LYS:CE    | 51:1:686:U:H5''  | 2.36                     | 0.48              |
| 29:G:116:LEU:HB3  | 29:G:140:LEU:CD2 | 2.43                     | 0.48              |
| 36:N:112:ARG:NH2  | 37:O:64:GLN:OE1  | 2.47                     | 0.48              |
| 42:T:50:HIS:CE1   | 50:3:667:G:H4'   | 2.49                     | 0.48              |
| 46:X:16:LYS:HE2   | 50:3:1012:A:OP2  | 2.14                     | 0.48              |
| 47:Y:30:PHE:O     | 47:Y:34:VAL:HG23 | 2.13                     | 0.48              |
| 50:3:938:A:C2     | 50:3:1376:U:H1'  | 2.49                     | 0.48              |
| 50:3:1424:U:H2'   | 50:3:1425:U:O4'  | 2.13                     | 0.48              |
| 51:1:1020:A:C1'   | 51:1:1021:A:OP2  | 2.56                     | 0.48              |
| 51:1:1721:G:H21   | 51:1:1722:A:N6   | 2.11                     | 0.48              |
| 51:1:2248:C:H2'   | 51:1:2249:U:H5'  | 1.95                     | 0.48              |
| 51:1:2599:G:H2'   | 51:1:2600:A:H8   | 1.79                     | 0.48              |
| 51:1:2637:U:H2'   | 51:1:2638:G:O4'  | 2.14                     | 0.48              |
| 52:2:78:A:H2'     | 52:2:79:G:O4'    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 55:8:139:THR:HA  | 55:8:142:GLN:OE1  | 2.13                     | 0.48              |
| 1:b:134:ILE:O    | 1:b:166:ARG:NH2   | 2.47                     | 0.48              |
| 1:b:229:HIS:CE1  | 1:b:230:PRO:HD2   | 2.49                     | 0.48              |
| 13:p:90:ALA:HB2  | 13:p:112:ARG:HG2  | 1.96                     | 0.48              |
| 27:E:55:GLY:O    | 27:E:58:ILE:HG22  | 2.14                     | 0.48              |
| 30:H:2:GLN:O     | 50:3:1190:G:H3'   | 2.13                     | 0.48              |
| 32:J:93:VAL:HG21 | 32:J:110:MET:CE   | 2.44                     | 0.48              |
| 36:N:98:ARG:NE   | 36:N:103:VAL:HG21 | 2.29                     | 0.48              |
| 47:Y:67:HIS:O    | 47:Y:69:ASN:N     | 2.47                     | 0.48              |
| 50:3:518:C:H4'   | 50:3:519:C:H5''   | 1.95                     | 0.48              |
| 50:3:1524:C:H2'  | 50:3:1525:G:C8    | 2.49                     | 0.48              |
| 51:1:569:U:C2'   | 51:1:570:G:H5'    | 2.44                     | 0.48              |
| 51:1:581:C:H2'   | 51:1:582:A:H8     | 1.77                     | 0.48              |
| 51:1:598:U:H2'   | 51:1:599:A:C8     | 2.49                     | 0.48              |
| 51:1:845:A:C3'   | 51:1:846:U:H5''   | 2.43                     | 0.48              |
| 51:1:2457:U:H5   | 51:1:2494:G:H1    | 1.60                     | 0.48              |
| 55:8:69:THR:O    | 55:8:109:LYS:HD3  | 2.13                     | 0.48              |
| 1:b:16:VAL:H     | 1:b:203:VAL:HG13  | 1.78                     | 0.48              |
| 1:b:158:GLY:H    | 1:b:194:VAL:HG13  | 1.77                     | 0.48              |
| 2:c:8:LYS:HB2    | 2:c:201:LEU:CD1   | 2.44                     | 0.48              |
| 2:c:104:VAL:HG22 | 2:c:105:LYS:N     | 2.28                     | 0.48              |
| 2:c:123:LYS:HZ3  | 51:1:2724:U:H5''  | 1.79                     | 0.48              |
| 3:d:162:ARG:NH1  | 51:1:340:A:O2'    | 2.45                     | 0.48              |
| 6:g:40:THR:O     | 6:g:44:ILE:HG12   | 2.14                     | 0.48              |
| 9:l:123:ARG:HA   | 9:l:144:GLU:HA    | 1.96                     | 0.48              |
| 11:n:92:GLY:O    | 51:1:2880:C:H1'   | 2.14                     | 0.48              |
| 12:o:12:THR:OG1  | 51:1:2334:U:H4'   | 2.14                     | 0.48              |
| 15:r:9:GLY:C     | 15:r:10:LYS:HD2   | 2.38                     | 0.48              |
| 19:v:2:PHE:HB3   | 19:v:50:MET:CE    | 2.44                     | 0.48              |
| 28:F:18:LYS:HG3  | 28:F:18:LYS:O     | 2.13                     | 0.48              |
| 32:J:149:PRO:O   | 32:J:152:VAL:HG22 | 2.14                     | 0.48              |
| 33:K:12:PRO:HB3  | 33:K:44:ARG:NH1   | 2.21                     | 0.48              |
| 33:K:15:SER:O    | 33:K:18:VAL:HG22  | 2.14                     | 0.48              |
| 33:K:18:VAL:H    | 33:K:19:PRO:HD3   | 1.76                     | 0.48              |
| 33:K:45:ARG:HG2  | 33:K:59:TYR:HD2   | 1.79                     | 0.48              |
| 34:L:131:GLY:O   | 34:L:135:LYS:HG3  | 2.14                     | 0.48              |
| 39:Q:86:VAL:HG23 | 39:Q:89:LEU:H     | 1.79                     | 0.48              |
| 44:V:18:LYS:HD2  | 44:V:48:GLU:O     | 2.13                     | 0.48              |
| 50:3:460:A:H2'   | 50:3:461:A:C8     | 2.48                     | 0.48              |
| 51:1:174:U:H2'   | 51:1:175:G:C8     | 2.48                     | 0.48              |
| 51:1:433:C:O2'   | 51:1:434:U:H5'    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 51:1:940:G:H2'   | 51:1:941:A:C5'    | 2.43                     | 0.48              |
| 51:1:940:G:C3'   | 51:1:941:A:H5''   | 2.44                     | 0.48              |
| 51:1:971:G:H2'   | 51:1:972:A:O4'    | 2.14                     | 0.48              |
| 51:1:1866:A:H2'  | 51:1:1867:G:O4'   | 2.13                     | 0.48              |
| 51:1:2105:U:O2'  | 51:1:2106:U:H5'   | 2.13                     | 0.48              |
| 51:1:2457:U:O2'  | 51:1:2458:G:H5'   | 2.14                     | 0.48              |
| 54:4:21:A:N1     | 55:8:213:ARG:HG3  | 2.28                     | 0.48              |
| 3:d:147:LEU:HB3  | 3:d:186:VAL:HG12  | 1.96                     | 0.48              |
| 4:e:3:LEU:CD2    | 4:e:100:GLU:HB3   | 2.44                     | 0.48              |
| 11:n:79:LEU:C    | 11:n:81:ASN:H     | 2.21                     | 0.48              |
| 15:r:7:SER:HB2   | 15:r:22:LEU:HD12  | 1.96                     | 0.48              |
| 29:G:69:VAL:HB   | 29:G:162:VAL:HG13 | 1.96                     | 0.48              |
| 29:G:113:LEU:CD2 | 29:G:151:LYS:HE2  | 2.43                     | 0.48              |
| 31:I:142:VAL:O   | 31:I:178:GLU:HG2  | 2.14                     | 0.48              |
| 33:K:90:MET:CE   | 45:W:60:ARG:HD3   | 2.44                     | 0.48              |
| 37:O:48:ARG:HH11 | 50:3:1368:A:H4'   | 1.79                     | 0.48              |
| 38:P:126:ARG:NH2 | 50:3:692:U:OP1    | 2.47                     | 0.48              |
| 50:3:701:U:C4'   | 50:3:703:G:H1'    | 2.44                     | 0.48              |
| 51:1:548:G:C2'   | 51:1:549:G:H4'    | 2.36                     | 0.48              |
| 51:1:2504:U:H2'  | 51:1:2505:G:H5''  | 1.95                     | 0.48              |
| 52:2:33:G:H2'    | 52:2:34:A:O4'     | 2.14                     | 0.48              |
| 7:j:13:ARG:HG2   | 7:j:13:ARG:NH2    | 2.28                     | 0.48              |
| 8:k:7:MET:C      | 8:k:8:LEU:HD12    | 2.38                     | 0.48              |
| 11:n:49:GLU:OE1  | 51:1:2839:G:H4'   | 2.14                     | 0.48              |
| 29:G:8:MET:HB3   | 29:G:13:VAL:HG21  | 1.95                     | 0.48              |
| 30:H:18:ASN:OD1  | 30:H:19:SER:N     | 2.47                     | 0.48              |
| 35:M:90:GLU:O    | 35:M:92:PRO:HD3   | 2.14                     | 0.48              |
| 35:M:105:THR:HB  | 35:M:120:LEU:HD11 | 1.95                     | 0.48              |
| 40:R:32:ILE:HG23 | 40:R:58:GLU:HB3   | 1.95                     | 0.48              |
| 50:3:159:G:H1'   | 50:3:162:A:H61    | 1.77                     | 0.48              |
| 50:3:865:A:H5'   | 50:3:1078:U:O4    | 2.14                     | 0.48              |
| 50:3:1325:C:O2'  | 50:3:1326:U:H5'   | 2.14                     | 0.48              |
| 50:3:1402:C:H2'  | 50:3:1403:C:O4'   | 2.12                     | 0.48              |
| 51:1:184:C:H2'   | 51:1:185:G:H8     | 1.78                     | 0.48              |
| 51:1:230:G:O2'   | 51:1:231:A:H5'    | 2.14                     | 0.48              |
| 51:1:347:A:H2'   | 51:1:348:A:H8     | 1.78                     | 0.48              |
| 51:1:368:A:O2'   | 51:1:369:U:H5'    | 2.14                     | 0.48              |
| 51:1:438:G:H2'   | 51:1:439:A:H8     | 1.78                     | 0.48              |
| 51:1:1409:U:H2'  | 51:1:1410:G:C8    | 2.49                     | 0.48              |
| 53:5:29:G:H2'    | 53:5:30:G:C8      | 2.49                     | 0.48              |
| 55:8:33:ARG:NH1  | 55:8:36:GLU:HB3   | 2.28                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:d:79:ARG:NH2    | 51:1:448:U:H4'    | 2.28                     | 0.47              |
| 5:f:132:LEU:HD12  | 5:f:132:LEU:O     | 2.14                     | 0.47              |
| 11:n:49:GLU:N     | 11:n:50:PRO:HD2   | 2.29                     | 0.47              |
| 15:r:7:SER:HB3    | 15:r:12:HIS:HD2   | 1.79                     | 0.47              |
| 17:t:29:THR:HG23  | 17:t:85:VAL:C     | 2.39                     | 0.47              |
| 27:E:39:ARG:O     | 27:E:43:LEU:HD23  | 2.13                     | 0.47              |
| 29:G:129:THR:CG2  | 29:G:132:GLU:HB3  | 2.44                     | 0.47              |
| 37:O:37:ARG:HG3   | 37:O:75:ASP:OD2   | 2.14                     | 0.47              |
| 40:R:27:THR:OG1   | 50:3:1329:A:P     | 2.72                     | 0.47              |
| 44:V:35:LYS:HG3   | 44:V:36:PHE:N     | 2.29                     | 0.47              |
| 50:3:556:C:H2'    | 50:3:557:G:C8     | 2.49                     | 0.47              |
| 50:3:1218:C:H2'   | 50:3:1219:A:C8    | 2.49                     | 0.47              |
| 50:3:1287:A:H2'   | 50:3:1288:A:C8    | 2.49                     | 0.47              |
| 50:3:1369:C:H2'   | 50:3:1370:G:H8    | 1.78                     | 0.47              |
| 51:1:1721:G:N2    | 51:1:1738:G:H1'   | 2.29                     | 0.47              |
| 51:1:2173:A:H2'   | 51:1:2173:A:N3    | 2.28                     | 0.47              |
| 51:1:2327:A:H2'   | 51:1:2328:A:C8    | 2.49                     | 0.47              |
| 51:1:2780:G:O2'   | 51:1:2781:A:H5'   | 2.13                     | 0.47              |
| 51:1:2800:A:H3'   | 51:1:2801:G:C5'   | 2.26                     | 0.47              |
| 52:2:55:U:H2'     | 52:2:56:G:C8      | 2.49                     | 0.47              |
| 55:8:50:PRO:HG2   | 55:8:51:GLU:H     | 1.79                     | 0.47              |
| 55:8:162:LYS:HD2  | 55:8:163:THR:N    | 2.29                     | 0.47              |
| 4:e:100:GLU:O     | 4:e:104:THR:OG1   | 2.30                     | 0.47              |
| 6:g:127:GLU:N     | 6:g:127:GLU:OE1   | 2.47                     | 0.47              |
| 10:m:81:ARG:HD3   | 51:1:2251:G:OP1   | 2.14                     | 0.47              |
| 14:q:77:LYS:O     | 14:q:116:LEU:HD11 | 2.14                     | 0.47              |
| 16:s:47:VAL:O     | 16:s:50:VAL:HG12  | 2.14                     | 0.47              |
| 19:v:44:HIS:O     | 19:v:47:VAL:HG22  | 2.14                     | 0.47              |
| 23:z:50:VAL:HA    | 23:z:52:PHE:CE1   | 2.48                     | 0.47              |
| 27:E:8:GLY:O      | 27:E:12:ARG:NH2   | 2.47                     | 0.47              |
| 29:G:73:ARG:HG3   | 29:G:73:ARG:HH11  | 1.79                     | 0.47              |
| 29:G:199:ILE:HD12 | 29:G:199:ILE:N    | 2.30                     | 0.47              |
| 32:J:112:ALA:O    | 32:J:115:GLU:HG2  | 2.13                     | 0.47              |
| 39:Q:113:ARG:NH1  | 50:3:36:C:H4'     | 2.29                     | 0.47              |
| 40:R:88:LEU:HA    | 40:R:91:ARG:HE    | 1.78                     | 0.47              |
| 41:S:48:GLN:HB2   | 46:X:12:LEU:HD22  | 1.95                     | 0.47              |
| 50:3:271:C:H2'    | 50:3:272:C:C6     | 2.49                     | 0.47              |
| 50:3:412:A:N6     | 50:3:431:A:H61    | 2.12                     | 0.47              |
| 50:3:545:C:H2'    | 50:3:546:A:O4'    | 2.14                     | 0.47              |
| 50:3:883:C:O2'    | 50:3:884:U:H5'    | 2.14                     | 0.47              |
| 51:1:2189:U:H2'   | 51:1:2190:G:H8    | 1.78                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 51:1:2249:U:O2'  | 51:1:2250:G:H5''  | 2.14                     | 0.47              |
| 51:1:2266:A:H4'  | 51:1:2267:A:N3    | 2.29                     | 0.47              |
| 52:2:41:G:H5'    | 52:2:42:C:H5''    | 1.95                     | 0.47              |
| 53:5:62:C:H2'    | 53:5:63:G:C8      | 2.48                     | 0.47              |
| 3:d:1:MET:N      | 3:d:14:VAL:O      | 2.47                     | 0.47              |
| 5:f:39:ALA:HA    | 5:f:57:TYR:CD2    | 2.49                     | 0.47              |
| 5:f:84:LYS:HB2   | 5:f:132:LEU:HD11  | 1.96                     | 0.47              |
| 12:o:10:ARG:HD3  | 51:1:2295:C:OP2   | 2.13                     | 0.47              |
| 29:G:216:VAL:O   | 29:G:219:THR:HG22 | 2.14                     | 0.47              |
| 31:I:72:ARG:NH1  | 31:I:203:TYR:HB3  | 2.29                     | 0.47              |
| 32:J:108:GLY:H   | 50:3:9:G:C4'      | 2.26                     | 0.47              |
| 36:N:70:GLY:O    | 36:N:74:GLN:HG3   | 2.14                     | 0.47              |
| 38:P:40:ALA:CB   | 50:3:706:A:H2     | 2.26                     | 0.47              |
| 38:P:86:LYS:CD   | 38:P:114:PRO:HD3  | 2.44                     | 0.47              |
| 41:S:69:PRO:HG2  | 41:S:70:HIS:ND1   | 2.29                     | 0.47              |
| 50:3:687:A:OP2   | 50:3:687:A:H8     | 1.98                     | 0.47              |
| 50:3:824:G:H2'   | 50:3:825:A:H8     | 1.79                     | 0.47              |
| 51:1:49:A:H5''   | 51:1:51:G:H5'     | 1.95                     | 0.47              |
| 51:1:1889:A:H2'  | 51:1:1890:A:C8    | 2.50                     | 0.47              |
| 51:1:2175:C:H2'  | 51:1:2176:A:C8    | 2.48                     | 0.47              |
| 51:1:2809:A:H2'  | 51:1:2809:A:N3    | 2.29                     | 0.47              |
| 5:f:108:PHE:HA   | 51:1:2666:C:H42   | 1.79                     | 0.47              |
| 6:g:94:ILE:HB    | 6:g:98:ASP:OD2    | 2.15                     | 0.47              |
| 8:k:28:SER:OG    | 51:1:2566:A:N1    | 2.46                     | 0.47              |
| 9:l:19:LEU:HD11  | 9:l:31:GLY:HA3    | 1.95                     | 0.47              |
| 9:l:126:ARG:HG2  | 9:l:126:ARG:NH2   | 2.29                     | 0.47              |
| 10:m:86:LYS:HA   | 51:1:956:G:OP1    | 2.14                     | 0.47              |
| 30:H:123:LEU:O   | 30:H:123:LEU:HD23 | 2.14                     | 0.47              |
| 32:J:130:THR:O   | 32:J:132:PRO:HD3  | 2.14                     | 0.47              |
| 34:L:39:GLU:OE1  | 36:N:42:THR:HG23  | 2.14                     | 0.47              |
| 41:S:8:ARG:HB3   | 41:S:12:ARG:HH12  | 1.79                     | 0.47              |
| 43:U:20:VAL:HG22 | 43:U:21:VAL:O     | 2.14                     | 0.47              |
| 46:X:10:ILE:HG13 | 46:X:11:ASP:N     | 2.24                     | 0.47              |
| 49:a:42:VAL:CG2  | 49:a:178:VAL:HG22 | 2.45                     | 0.47              |
| 50:3:1167:A:H2'  | 50:3:1167:A:N3    | 2.29                     | 0.47              |
| 50:3:1369:C:H2'  | 50:3:1370:G:C8    | 2.48                     | 0.47              |
| 50:3:1435:G:H2'  | 50:3:1436:U:C6    | 2.49                     | 0.47              |
| 50:3:1487:G:O2'  | 50:3:1488:G:H5'   | 2.15                     | 0.47              |
| 51:1:1138:G:H2'  | 51:1:1139:G:O4'   | 2.15                     | 0.47              |
| 51:1:1951:U:H2'  | 51:1:1953:A:OP2   | 2.14                     | 0.47              |
| 53:5:15:G:H22    | 53:5:48:C:N4      | 1.92                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:8:170:GLU:OE2  | 55:8:175:GLY:N    | 2.47                     | 0.47              |
| 1:b:52:HIS:CG     | 1:b:218:THR:HG22  | 2.48                     | 0.47              |
| 4:e:134:GLN:HB3   | 4:e:151:LEU:HD13  | 1.96                     | 0.47              |
| 13:p:21:PRO:HG3   | 13:p:94:ALA:HA    | 1.97                     | 0.47              |
| 14:q:7:VAL:HG11   | 51:1:1215:G:H5'   | 1.96                     | 0.47              |
| 16:s:106:VAL:HG13 | 16:s:106:VAL:O    | 2.14                     | 0.47              |
| 18:u:33:VAL:HG13  | 18:u:66:VAL:HG12  | 1.96                     | 0.47              |
| 28:F:25:VAL:HG21  | 28:F:35:GLN:HE21  | 1.80                     | 0.47              |
| 29:G:27:LYS:N     | 29:G:28:PRO:CD    | 2.77                     | 0.47              |
| 30:H:48:LYS:H     | 30:H:48:LYS:HD3   | 1.79                     | 0.47              |
| 38:P:35:ASP:OD1   | 38:P:39:ASN:N     | 2.47                     | 0.47              |
| 39:Q:14:LYS:NZ    | 50:3:562:U:H6     | 2.11                     | 0.47              |
| 45:W:54:LEU:O     | 45:W:58:ILE:HG13  | 2.14                     | 0.47              |
| 47:Y:2:ASN:HD22   | 47:Y:4:LYS:NZ     | 2.12                     | 0.47              |
| 49:a:5:THR:CG2    | 49:a:6:LYS:H      | 2.20                     | 0.47              |
| 49:a:46:VAL:HB    | 49:a:171:ILE:HD12 | 1.95                     | 0.47              |
| 50:3:273:U:C2'    | 50:3:274:A:H5'    | 2.44                     | 0.47              |
| 50:3:823:C:H2'    | 50:3:824:G:C8     | 2.49                     | 0.47              |
| 50:3:1420:U:H2'   | 50:3:1421:G:C8    | 2.49                     | 0.47              |
| 51:1:580:U:H2'    | 51:1:581:C:C6     | 2.49                     | 0.47              |
| 51:1:1524:G:H2'   | 51:1:1525:A:C8    | 2.50                     | 0.47              |
| 51:1:1548:A:H2'   | 51:1:1549:A:C8    | 2.49                     | 0.47              |
| 51:1:1825:U:H2'   | 51:1:1826:G:C8    | 2.49                     | 0.47              |
| 51:1:2220:U:H2'   | 51:1:2221:G:H8    | 1.80                     | 0.47              |
| 1:b:93:VAL:HG22   | 1:b:94:LEU:N      | 2.29                     | 0.47              |
| 2:c:8:LYS:HD2     | 2:c:193:VAL:HG23  | 1.96                     | 0.47              |
| 9:l:61:LEU:HD13   | 27:E:23:HIS:CG    | 2.49                     | 0.47              |
| 9:l:77:ILE:HD11   | 9:l:108:ALA:HB1   | 1.97                     | 0.47              |
| 11:n:93:GLY:HA3   | 51:1:2880:C:O2    | 2.14                     | 0.47              |
| 25:C:3:GLY:HA3    | 51:1:2284:A:P     | 2.55                     | 0.47              |
| 25:C:27:ARG:NE    | 25:C:27:ARG:HA    | 2.29                     | 0.47              |
| 30:H:6:PRO:HD2    | 30:H:183:TYR:CD2  | 2.49                     | 0.47              |
| 32:J:23:THR:HG21  | 50:3:15:G:H1'     | 1.95                     | 0.47              |
| 41:S:74:ARG:HB2   | 50:3:1358:U:OP1   | 2.15                     | 0.47              |
| 49:a:11:ILE:HG22  | 49:a:220:ALA:HB3  | 1.96                     | 0.47              |
| 50:3:20:U:H2'     | 50:3:21:G:O4'     | 2.15                     | 0.47              |
| 50:3:231:U:H2'    | 50:3:232:G:H8     | 1.80                     | 0.47              |
| 50:3:1260:G:H4'   | 50:3:1284:C:H5'   | 1.95                     | 0.47              |
| 50:3:1513:A:H2'   | 50:3:1514:G:C8    | 2.50                     | 0.47              |
| 51:1:402:A:H2'    | 51:1:403:U:O4'    | 2.15                     | 0.47              |
| 51:1:828:U:H4'    | 51:1:831:G:N1     | 2.29                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 51:1:1329:U:H5'' | 51:1:1330:C:OP2   | 2.14                     | 0.47              |
| 51:1:1689:A:H2'  | 51:1:1690:A:C8    | 2.49                     | 0.47              |
| 51:1:2391:G:H1   | 51:1:2424:C:H3'   | 1.78                     | 0.47              |
| 51:1:2440:C:C4   | 51:1:2441:U:H1'   | 2.50                     | 0.47              |
| 55:8:127:ASP:HB2 | 55:8:183:ILE:O    | 2.15                     | 0.47              |
| 55:8:159:ARG:HB3 | 55:8:161:PHE:CE2  | 2.48                     | 0.47              |
| 55:8:200:ARG:HD3 | 55:8:322:GLN:HB3  | 1.97                     | 0.47              |
| 2:c:121:THR:HB   | 2:c:127:PHE:CD2   | 2.49                     | 0.47              |
| 4:e:35:LEU:HD12  | 4:e:88:VAL:HG13   | 1.96                     | 0.47              |
| 4:e:42:ALA:O     | 4:e:46:LYS:HD3    | 2.14                     | 0.47              |
| 12:o:51:ALA:HB2  | 12:o:81:ARG:HD3   | 1.97                     | 0.47              |
| 13:p:24:THR:HG21 | 13:p:87:ARG:HG3   | 1.95                     | 0.47              |
| 14:q:1:ALA:HB1   | 51:1:445:C:OP1    | 2.14                     | 0.47              |
| 16:s:70:LYS:C    | 16:s:107:VAL:HG23 | 2.39                     | 0.47              |
| 17:t:61:LEU:N    | 17:t:61:LEU:HD23  | 2.30                     | 0.47              |
| 19:v:78:GLN:CB   | 19:v:88:HIS:HB3   | 2.45                     | 0.47              |
| 21:x:21:LEU:O    | 51:1:200:U:H5''   | 2.15                     | 0.47              |
| 21:x:38:TRP:HB2  | 21:x:45:PHE:CE1   | 2.50                     | 0.47              |
| 26:D:21:ARG:NH1  | 51:1:466:A:H5'    | 2.30                     | 0.47              |
| 33:K:22:ILE:HA   | 33:K:25:TYR:CD2   | 2.50                     | 0.47              |
| 38:P:124:LYS:HD3 | 48:Z:34:ARG:HA    | 1.97                     | 0.47              |
| 40:R:28:ARG:HB2  | 50:3:1329:A:OP1   | 2.15                     | 0.47              |
| 49:a:166:ASP:HB2 | 51:1:2122:U:O2    | 2.15                     | 0.47              |
| 49:a:215:SER:CB  | 51:1:2176:A:H1'   | 2.37                     | 0.47              |
| 50:3:224:U:H2'   | 50:3:225:C:C6     | 2.50                     | 0.47              |
| 50:3:323:U:H2'   | 50:3:324:G:O4'    | 2.15                     | 0.47              |
| 50:3:1205:U:H2'  | 50:3:1206:G:H8    | 1.79                     | 0.47              |
| 50:3:1442:G:H2'  | 50:3:1442:G:N3    | 2.28                     | 0.47              |
| 50:3:1492:A:C2   | 54:4:21:A:H5''    | 2.49                     | 0.47              |
| 51:1:60:G:O2'    | 51:1:61:C:H5''    | 2.15                     | 0.47              |
| 51:1:100:U:H4'   | 51:1:101:A:C4     | 2.49                     | 0.47              |
| 51:1:1553:A:H2'  | 51:1:1553:A:N3    | 2.29                     | 0.47              |
| 51:1:1639:C:O2'  | 51:1:1640:A:H5'   | 2.14                     | 0.47              |
| 51:1:1859:U:H2'  | 51:1:1860:G:C8    | 2.49                     | 0.47              |
| 51:1:2039:U:H2'  | 51:1:2040:G:H8    | 1.79                     | 0.47              |
| 51:1:2324:U:H4'  | 51:1:2337:G:H5''  | 1.97                     | 0.47              |
| 55:8:264:THR:CA  | 55:8:291:MET:HE1  | 2.44                     | 0.47              |
| 1:b:32:LEU:HD11  | 1:b:101:ARG:HA    | 1.95                     | 0.47              |
| 1:b:183:VAL:HG22 | 1:b:184:GLU:N     | 2.30                     | 0.47              |
| 1:b:220:ARG:NH2  | 1:b:237:ARG:HH21  | 2.08                     | 0.47              |
| 1:b:269:ARG:HG3  | 1:b:269:ARG:HH11  | 1.79                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:d:77:ILE:HD13  | 51:l:673:C:H4'    | 1.96                     | 0.47              |
| 10:m:42:THR:HA   | 10:m:93:VAL:HG12  | 1.96                     | 0.47              |
| 12:o:3:LYS:NZ    | 52:2:46:A:H5''    | 2.30                     | 0.47              |
| 13:p:32:VAL:HG12 | 13:p:37:LYS:HA    | 1.97                     | 0.47              |
| 18:u:44:HIS:HB2  | 51:l:482:A:H4'    | 1.97                     | 0.47              |
| 21:x:42:GLU:CB   | 21:x:44:ARG:HG2   | 2.45                     | 0.47              |
| 34:L:113:LYS:HB2 | 34:L:117:LEU:HD23 | 1.96                     | 0.47              |
| 34:L:132:THR:HA  | 34:L:135:LYS:CD   | 2.39                     | 0.47              |
| 36:N:119:LYS:HG3 | 50:3:1349:A:OP1   | 2.15                     | 0.47              |
| 39:Q:5:GLN:NE2   | 50:3:880:C:H3'    | 2.29                     | 0.47              |
| 40:R:22:TYR:OH   | 40:R:72:ILE:HD12  | 2.14                     | 0.47              |
| 48:Z:8:ASN:CG    | 48:Z:9:GLU:H      | 2.22                     | 0.47              |
| 50:3:477:C:H2'   | 50:3:478:A:C8     | 2.49                     | 0.47              |
| 50:3:558:G:H2'   | 50:3:559:A:C2     | 2.50                     | 0.47              |
| 51:l:197:A:H4'   | 51:l:2069:G:OP1   | 2.14                     | 0.47              |
| 51:l:435:C:H2'   | 51:l:436:C:H5'    | 1.96                     | 0.47              |
| 51:l:813:U:H2'   | 51:l:814:C:C6     | 2.50                     | 0.47              |
| 51:l:1479:G:C4'  | 51:l:1560:G:H21   | 2.27                     | 0.47              |
| 51:l:2443:C:H2'  | 51:l:2444:G:H8    | 1.79                     | 0.47              |
| 51:l:2533:U:OP1  | 51:l:2665:A:H1'   | 2.15                     | 0.47              |
| 1:b:110:LYS:N    | 1:b:113:ASP:OD2   | 2.44                     | 0.47              |
| 2:c:142:VAL:HG23 | 2:c:143:PRO:HD2   | 1.97                     | 0.47              |
| 5:f:171:LYS:HE3  | 51:l:2529:G:OP2   | 2.13                     | 0.47              |
| 7:j:4:PHE:O      | 14:q:63:ARG:NH1   | 2.46                     | 0.47              |
| 10:m:33:LEU:HD11 | 10:m:128:THR:OG1  | 2.14                     | 0.47              |
| 11:n:31:HIS:C    | 11:n:33:ILE:H     | 2.23                     | 0.47              |
| 12:o:15:ARG:O    | 12:o:19:GLN:N     | 2.48                     | 0.47              |
| 12:o:111:ARG:HG2 | 12:o:111:ARG:NH2  | 2.29                     | 0.47              |
| 13:p:105:LYS:HD2 | 13:p:108:ARG:NH1  | 2.29                     | 0.47              |
| 19:v:1:MET:HB3   | 19:v:59:GLU:OE1   | 2.15                     | 0.47              |
| 21:x:63:ILE:HG23 | 21:x:64:ASP:N     | 2.30                     | 0.47              |
| 25:C:46:VAL:HG12 | 25:C:47:ILE:N     | 2.29                     | 0.47              |
| 30:H:155:ARG:NE  | 30:H:159:ALA:O    | 2.46                     | 0.47              |
| 30:H:173:PRO:HA  | 50:3:1108:G:OP2   | 2.15                     | 0.47              |
| 33:K:6:ILE:HD13  | 33:K:74:LEU:HD23  | 1.97                     | 0.47              |
| 37:O:47:GLU:CB   | 37:O:67:ILE:HB    | 2.42                     | 0.47              |
| 39:Q:73:LEU:HA   | 39:Q:76:HIS:CE1   | 2.50                     | 0.47              |
| 40:R:64:VAL:HG23 | 40:R:67:ASP:H     | 1.80                     | 0.47              |
| 41:S:74:ARG:NH2  | 50:3:1360:A:OP2   | 2.47                     | 0.47              |
| 42:T:79:GLN:HE22 | 42:T:83:ARG:HB2   | 1.79                     | 0.47              |
| 46:X:71:GLY:HA3  | 50:3:1320:C:O2    | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 50:3:5:U:H4'     | 50:3:6:G:C8      | 2.49                     | 0.47              |
| 50:3:882:C:O2'   | 50:3:883:C:H5'   | 2.15                     | 0.47              |
| 51:1:225:C:H2'   | 51:1:226:A:O4'   | 2.14                     | 0.47              |
| 51:1:1023:U:O2'  | 51:1:1122:G:H5'  | 2.15                     | 0.47              |
| 51:1:1670:C:O5'  | 51:1:1670:C:H6   | 1.98                     | 0.47              |
| 51:1:1755:A:H2'  | 51:1:1756:G:H5'  | 1.95                     | 0.47              |
| 51:1:1935:G:H2'  | 51:1:1962:C:H42  | 1.80                     | 0.47              |
| 52:2:12:C:H1'    | 52:2:15:A:N6     | 2.30                     | 0.47              |
| 55:8:46:VAL:O    | 55:8:46:VAL:HG12 | 2.15                     | 0.47              |
| 1:b:230:PRO:O    | 1:b:241:LYS:HE3  | 2.15                     | 0.47              |
| 2:c:173:GLN:NE2  | 2:c:208:LYS:HZ2  | 2.13                     | 0.47              |
| 5:f:116:LEU:CD1  | 5:f:143:VAL:HG21 | 2.45                     | 0.47              |
| 11:n:117:ASP:O   | 11:n:118:ARG:C   | 2.58                     | 0.47              |
| 14:q:57:ARG:O    | 14:q:61:ILE:HG12 | 2.15                     | 0.47              |
| 18:u:6:ARG:O     | 18:u:24:VAL:HB   | 2.14                     | 0.47              |
| 34:L:58:LEU:HD12 | 34:L:58:LEU:N    | 2.27                     | 0.47              |
| 35:M:4:ASP:OD2   | 35:M:7:ALA:HB3   | 2.15                     | 0.47              |
| 36:N:6:TYR:OH    | 50:3:1148:U:H5'  | 2.14                     | 0.47              |
| 36:N:21:LYS:HB3  | 36:N:22:PRO:HD2  | 1.96                     | 0.47              |
| 36:N:40:ARG:HG2  | 36:N:41:GLU:OE2  | 2.14                     | 0.47              |
| 37:O:76:ILE:HG22 | 37:O:78:GLU:HG2  | 1.96                     | 0.47              |
| 38:P:124:LYS:HZ2 | 48:Z:34:ARG:HA   | 1.80                     | 0.47              |
| 42:T:42:PHE:CE2  | 42:T:55:LEU:HD22 | 2.50                     | 0.47              |
| 47:Y:35:TYR:HD1  | 47:Y:38:ILE:HD12 | 1.80                     | 0.47              |
| 50:3:1346:A:C2'  | 50:3:1347:G:H4'  | 2.43                     | 0.47              |
| 50:3:1404:C:H2'  | 50:3:1405:G:H8   | 1.80                     | 0.47              |
| 51:1:5:A:H2'     | 51:1:6:A:C8      | 2.49                     | 0.47              |
| 51:1:186:G:H2'   | 51:1:187:G:H8    | 1.80                     | 0.47              |
| 51:1:204:A:O3'   | 51:1:205:G:H4'   | 2.16                     | 0.47              |
| 51:1:2366:A:H2'  | 51:1:2367:G:O4'  | 2.15                     | 0.47              |
| 51:1:2504:U:H3'  | 51:1:2505:G:H5'' | 1.96                     | 0.47              |
| 1:b:64:VAL:HG13  | 1:b:66:PHE:HD1   | 1.80                     | 0.46              |
| 4:e:114:ARG:NE   | 4:e:175:PRO:HD2  | 2.29                     | 0.46              |
| 4:e:149:ARG:HG2  | 4:e:149:ARG:HH11 | 1.80                     | 0.46              |
| 10:m:16:ARG:HG2  | 10:m:16:ARG:HH11 | 1.80                     | 0.46              |
| 12:o:76:LYS:O    | 12:o:80:GLU:N    | 2.42                     | 0.46              |
| 13:p:50:ARG:HH22 | 51:1:2683:C:H5'' | 1.80                     | 0.46              |
| 14:q:20:ALA:HA   | 14:q:23:TYR:CE2  | 2.50                     | 0.46              |
| 26:D:34:ARG:NH2  | 51:1:466:A:OP1   | 2.49                     | 0.46              |
| 32:J:104:ILE:CD1 | 32:J:122:VAL:HB  | 2.45                     | 0.46              |
| 36:N:5:TYR:CD2   | 36:N:20:ILE:HG23 | 2.47                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 36:N:11:ARG:HH22 | 36:N:108:ARG:CD   | 2.28                     | 0.46              |
| 36:N:46:VAL:O    | 36:N:79:ARG:HD3   | 2.15                     | 0.46              |
| 37:O:15:HIS:CD2  | 50:3:1152:A:H5'   | 2.50                     | 0.46              |
| 39:Q:14:LYS:HZ1  | 50:3:562:U:H6     | 1.63                     | 0.46              |
| 46:X:10:ILE:O    | 46:X:11:ASP:CG    | 2.58                     | 0.46              |
| 51:1:84:A:H4'    | 51:1:85:G:O5'     | 2.15                     | 0.46              |
| 51:1:347:A:H2'   | 51:1:348:A:C8     | 2.50                     | 0.46              |
| 51:1:479:A:C4'   | 51:1:480:A:H5'    | 2.45                     | 0.46              |
| 51:1:1437:C:H2'  | 51:1:1438:U:C6    | 2.49                     | 0.46              |
| 51:1:2149:U:H2'  | 51:1:2150:C:O4'   | 2.14                     | 0.46              |
| 1:b:129:LEU:N    | 1:b:129:LEU:HD23  | 2.30                     | 0.46              |
| 1:b:257:ARG:HH12 | 1:b:263:ASP:HB3   | 1.81                     | 0.46              |
| 5:f:84:LYS:HB2   | 5:f:132:LEU:CD1   | 2.46                     | 0.46              |
| 6:g:62:LEU:HD23  | 6:g:62:LEU:C      | 2.40                     | 0.46              |
| 13:p:24:THR:HG22 | 13:p:87:ARG:HG3   | 1.95                     | 0.46              |
| 31:I:31:CYS:SG   | 31:I:32:LYS:N     | 2.89                     | 0.46              |
| 31:I:99:ASN:ND2  | 31:I:110:ARG:HH21 | 2.14                     | 0.46              |
| 34:L:110:ARG:HD3 | 34:L:122:GLU:OE2  | 2.15                     | 0.46              |
| 36:N:9:GLY:C     | 36:N:10:ARG:HD3   | 2.40                     | 0.46              |
| 36:N:83:THR:HA   | 36:N:86:LEU:HD12  | 1.95                     | 0.46              |
| 38:P:45:THR:OG1  | 38:P:48:GLY:HA3   | 2.16                     | 0.46              |
| 38:P:58:THR:HG23 | 38:P:61:ALA:H     | 1.80                     | 0.46              |
| 39:Q:38:THR:HG23 | 39:Q:49:ARG:O     | 2.15                     | 0.46              |
| 40:R:63:VAL:HG23 | 40:R:67:ASP:OD2   | 2.16                     | 0.46              |
| 41:S:30:ILE:HD12 | 41:S:30:ILE:N     | 2.30                     | 0.46              |
| 41:S:58:ARG:HH21 | 50:3:980:C:C4'    | 2.27                     | 0.46              |
| 41:S:60:ARG:NH1  | 50:3:981:U:O2'    | 2.48                     | 0.46              |
| 45:W:12:PHE:CD2  | 45:W:13:THR:HG22  | 2.50                     | 0.46              |
| 49:a:189:LEU:O   | 49:a:193:LEU:N    | 2.48                     | 0.46              |
| 50:3:350:G:H2'   | 50:3:351:G:C8     | 2.50                     | 0.46              |
| 50:3:1495:U:H2'  | 50:3:1496:C:C6    | 2.51                     | 0.46              |
| 51:1:406:G:H2'   | 51:1:407:G:C8     | 2.50                     | 0.46              |
| 51:1:700:G:O2'   | 51:1:701:G:H5'    | 2.15                     | 0.46              |
| 51:1:2066:C:O2'  | 51:1:2067:G:H5'   | 2.14                     | 0.46              |
| 51:1:2069:G:O2'  | 51:1:2070:A:H5'   | 2.16                     | 0.46              |
| 6:g:12:LEU:HG    | 51:1:2095:A:OP1   | 2.15                     | 0.46              |
| 7:j:15:TRP:HH2   | 51:1:7:G:H4'      | 1.80                     | 0.46              |
| 8:k:32:TYR:OH    | 51:1:1996:C:H5    | 1.99                     | 0.46              |
| 11:n:10:LEU:O    | 11:n:12:ARG:HG3   | 2.15                     | 0.46              |
| 15:r:1:MET:N     | 15:r:43:ASN:HA    | 2.30                     | 0.46              |
| 19:v:14:LYS:HB2  | 52:2:98:G:H1      | 1.81                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:G:118:THR:HG23 | 29:G:119:GLN:HE21 | 1.78                     | 0.46              |
| 30:H:47:ALA:HA    | 30:H:51:VAL:HG12  | 1.98                     | 0.46              |
| 40:R:114:PRO:O    | 50:3:1228:C:H4'   | 2.16                     | 0.46              |
| 50:3:291:U:H2'    | 50:3:292:G:C8     | 2.50                     | 0.46              |
| 50:3:911:U:H2'    | 50:3:912:C:C6     | 2.50                     | 0.46              |
| 51:1:49:A:C5'     | 51:1:51:G:H5'     | 2.45                     | 0.46              |
| 51:1:325:G:H2'    | 51:1:326:G:H8     | 1.81                     | 0.46              |
| 51:1:1555:G:H2'   | 51:1:1556:C:C6    | 2.50                     | 0.46              |
| 51:1:1668:A:C4'   | 51:1:1669:A:H5'   | 2.42                     | 0.46              |
| 51:1:2849:U:H4'   | 51:1:2868:A:C2    | 2.50                     | 0.46              |
| 55:8:72:GLN:O     | 55:8:76:GLY:N     | 2.48                     | 0.46              |
| 1:b:7:PRO:HB3     | 1:b:13:ARG:HA     | 1.96                     | 0.46              |
| 1:b:68:ARG:CD     | 1:b:103:ILE:HD12  | 2.45                     | 0.46              |
| 1:b:184:GLU:HG3   | 1:b:186:ASP:H     | 1.79                     | 0.46              |
| 3:d:104:ALA:O     | 3:d:108:ILE:HG13  | 2.15                     | 0.46              |
| 5:f:2:ARG:HA      | 5:f:5:LYS:HE2     | 1.96                     | 0.46              |
| 12:o:4:LYS:O      | 12:o:8:ILE:HG13   | 2.15                     | 0.46              |
| 15:r:1:MET:H1     | 15:r:43:ASN:HA    | 1.80                     | 0.46              |
| 15:r:13:ARG:HD2   | 15:r:13:ARG:C     | 2.40                     | 0.46              |
| 15:r:27:ILE:CG2   | 15:r:28:ALA:H     | 2.18                     | 0.46              |
| 26:D:26:ASN:CG    | 51:1:682:G:H5'    | 2.40                     | 0.46              |
| 30:H:29:ALA:HB1   | 41:S:64:ARG:NH2   | 2.30                     | 0.46              |
| 31:I:186:GLU:HG2  | 31:I:189:ASP:OD2  | 2.15                     | 0.46              |
| 50:3:790:A:H5'    | 53:5:39:C:H5'     | 1.97                     | 0.46              |
| 51:1:2027:G:H2'   | 51:1:2028:U:C6    | 2.51                     | 0.46              |
| 51:1:2241:A:H2'   | 51:1:2242:G:C8    | 2.50                     | 0.46              |
| 55:8:33:ARG:NH2   | 55:8:40:GLU:OE2   | 2.43                     | 0.46              |
| 55:8:189:TYR:O    | 55:8:193:ARG:N    | 2.48                     | 0.46              |
| 2:c:23:PRO:HB3    | 51:1:2682:A:C2    | 2.50                     | 0.46              |
| 2:c:43:ASP:OD1    | 2:c:44:GLY:N      | 2.48                     | 0.46              |
| 3:d:68:ALA:HA     | 51:1:1255:U:C6    | 2.51                     | 0.46              |
| 5:f:46:ASP:C      | 5:f:48:THR:H      | 2.23                     | 0.46              |
| 6:g:3:VAL:HA      | 6:g:39:ALA:N      | 2.30                     | 0.46              |
| 7:j:31:GLU:HG3    | 7:j:142:ILE:HG13  | 1.97                     | 0.46              |
| 9:l:62:PRO:HB3    | 51:1:2393:U:H5''  | 1.97                     | 0.46              |
| 16:s:57:ASN:OD1   | 51:1:495:G:H1'    | 2.16                     | 0.46              |
| 19:v:65:VAL:O     | 19:v:65:VAL:HG13  | 2.16                     | 0.46              |
| 22:y:22:LEU:HD23  | 22:y:22:LEU:C     | 2.41                     | 0.46              |
| 25:C:25:ASN:HD21  | 25:C:28:THR:HG23  | 1.81                     | 0.46              |
| 27:E:2:LYS:HG2    | 51:1:592:A:H4'    | 1.97                     | 0.46              |
| 34:L:12:LEU:CD1   | 34:L:13:PRO:HD2   | 2.46                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:L:96:ASN:O    | 34:L:100:MET:HG3  | 2.15                     | 0.46              |
| 36:N:45:MET:HB3  | 36:N:48:ARG:NH2   | 2.26                     | 0.46              |
| 46:X:39:ILE:HG13 | 46:X:68:HIS:O     | 2.15                     | 0.46              |
| 47:Y:2:ASN:CG    | 47:Y:3:ILE:H      | 2.22                     | 0.46              |
| 50:3:990:C:H2'   | 50:3:991:U:O4'    | 2.15                     | 0.46              |
| 50:3:1490:U:O2'  | 50:3:1491:G:H5'   | 2.15                     | 0.46              |
| 51:1:1111:A:H2'  | 51:1:1112:G:C4'   | 2.45                     | 0.46              |
| 51:1:1319:C:O2'  | 51:1:1320:C:H5'   | 2.16                     | 0.46              |
| 51:1:1422:G:H2'  | 51:1:1423:G:C8    | 2.51                     | 0.46              |
| 51:1:1443:U:H2'  | 51:1:1444:G:H8    | 1.81                     | 0.46              |
| 51:1:2427:C:C5'  | 51:1:2429:G:H5'   | 2.45                     | 0.46              |
| 55:8:27:TYR:O    | 55:8:31:LYS:HD3   | 2.15                     | 0.46              |
| 2:c:122:VAL:HG11 | 2:c:141:ARG:HH21  | 1.81                     | 0.46              |
| 3:d:23:PHE:HB2   | 3:d:114:ARG:HH22  | 1.79                     | 0.46              |
| 3:d:134:LEU:HD23 | 3:d:164:LEU:HD12  | 1.97                     | 0.46              |
| 5:f:88:LEU:HD21  | 5:f:93:TYR:HB3    | 1.98                     | 0.46              |
| 6:g:121:VAL:HG22 | 6:g:121:VAL:O     | 2.15                     | 0.46              |
| 9:l:58:TYR:O     | 27:E:12:ARG:HD2   | 2.16                     | 0.46              |
| 13:p:57:ALA:HA   | 13:p:75:THR:HG23  | 1.96                     | 0.46              |
| 14:q:40:LYS:HG3  | 14:q:44:TYR:CE2   | 2.49                     | 0.46              |
| 32:J:84:VAL:HG22 | 32:J:85:LYS:N     | 2.31                     | 0.46              |
| 32:J:96:GLN:N    | 32:J:123:LEU:O    | 2.45                     | 0.46              |
| 34:L:92:PRO:HA   | 34:L:95:ARG:HE    | 1.79                     | 0.46              |
| 39:Q:50:LYS:HB3  | 39:Q:66:ILE:HB    | 1.97                     | 0.46              |
| 44:V:15:LYS:HE3  | 50:3:275:G:H5'    | 1.97                     | 0.46              |
| 46:X:69:LYS:HE2  | 50:3:1319:A:H5''  | 1.98                     | 0.46              |
| 50:3:1491:G:H1'  | 50:3:1492:A:OP1   | 2.15                     | 0.46              |
| 51:1:1680:U:H2'  | 51:1:1681:G:H5'   | 1.98                     | 0.46              |
| 51:1:2428:G:H5'' | 51:1:2429:G:O5'   | 2.15                     | 0.46              |
| 52:2:49:C:H2'    | 52:2:50:A:C8      | 2.50                     | 0.46              |
| 6:g:17:ASP:OD1   | 6:g:17:ASP:N      | 2.48                     | 0.46              |
| 16:s:71:VAL:HG23 | 16:s:71:VAL:O     | 2.15                     | 0.46              |
| 16:s:88:ARG:HG3  | 16:s:94:ASP:OD2   | 2.16                     | 0.46              |
| 19:v:29:ILE:HD11 | 19:v:37:PRO:HB2   | 1.97                     | 0.46              |
| 20:w:62:LYS:HB2  | 20:w:79:GLU:HB2   | 1.98                     | 0.46              |
| 31:I:59:LYS:HZ2  | 31:I:194:ILE:HG22 | 1.79                     | 0.46              |
| 32:J:157:GLY:O   | 32:J:158:LYS:HB2  | 2.15                     | 0.46              |
| 36:N:48:ARG:O    | 36:N:52:GLU:HG3   | 2.16                     | 0.46              |
| 37:O:23:ALA:O    | 37:O:26:VAL:HG12  | 2.16                     | 0.46              |
| 43:U:28:ARG:NH2  | 43:U:29:ASN:HD21  | 2.14                     | 0.46              |
| 46:X:14:LEU:O    | 46:X:18:VAL:N     | 2.48                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:3:1060:U:H2'   | 50:3:1061:G:H8    | 1.80                     | 0.46              |
| 51:1:419:U:H2'    | 51:1:420:C:C6     | 2.51                     | 0.46              |
| 51:1:680:C:H2'    | 51:1:681:G:C8     | 2.50                     | 0.46              |
| 51:1:1328:A:H4'   | 51:1:1329:U:C5    | 2.51                     | 0.46              |
| 51:1:1421:G:H2'   | 51:1:1422:G:H8    | 1.80                     | 0.46              |
| 51:1:1566:A:O2'   | 51:1:1567:G:H5'   | 2.15                     | 0.46              |
| 3:d:47:LYS:O      | 3:d:83:VAL:HG23   | 2.16                     | 0.46              |
| 6:g:93:SER:CB     | 6:g:121:VAL:HG21  | 2.44                     | 0.46              |
| 11:n:56:LYS:HE3   | 11:n:87:PHE:O     | 2.16                     | 0.46              |
| 16:s:14:ALA:O     | 16:s:17:VAL:HG22  | 2.15                     | 0.46              |
| 18:u:80:ASP:OD2   | 18:u:96:LYS:N     | 2.49                     | 0.46              |
| 21:x:42:GLU:HB3   | 21:x:44:ARG:HG2   | 1.98                     | 0.46              |
| 29:G:137:THR:HA   | 29:G:140:LEU:HD12 | 1.98                     | 0.46              |
| 31:I:31:CYS:HB2   | 31:I:33:ILE:HD11  | 1.97                     | 0.46              |
| 34:L:15:PRO:HB3   | 36:N:43:ALA:HA    | 1.98                     | 0.46              |
| 36:N:28:VAL:HG13  | 36:N:63:TYR:HA    | 1.97                     | 0.46              |
| 38:P:118:ASN:HD22 | 50:3:718:A:C5'    | 2.29                     | 0.46              |
| 43:U:20:VAL:HG23  | 43:U:34:GLU:C     | 2.41                     | 0.46              |
| 43:U:40:ASN:HB3   | 43:U:43:ALA:HB2   | 1.97                     | 0.46              |
| 50:3:56:U:H2'     | 50:3:57:G:H8      | 1.81                     | 0.46              |
| 50:3:485:U:H5'    | 50:3:486:U:OP2    | 2.15                     | 0.46              |
| 51:1:1614:A:H2'   | 51:1:1615:C:H5'   | 1.97                     | 0.46              |
| 51:1:2751:G:H2'   | 51:1:2751:G:N3    | 2.31                     | 0.46              |
| 1:b:43:ASN:ND2    | 1:b:45:ASN:H      | 2.13                     | 0.46              |
| 2:c:161:MET:CE    | 51:1:2050:C:H1'   | 2.45                     | 0.46              |
| 3:d:122:GLU:CD    | 3:d:122:GLU:H     | 2.24                     | 0.46              |
| 5:f:174:LYS:HB2   | 51:1:2531:A:P     | 2.55                     | 0.46              |
| 6:g:8:LYS:HG3     | 6:g:8:LYS:O       | 2.15                     | 0.46              |
| 9:l:48:ARG:HG3    | 9:l:48:ARG:HH11   | 1.81                     | 0.46              |
| 10:m:29:GLY:O     | 10:m:133:LYS:HD3  | 2.16                     | 0.46              |
| 11:n:100:CYS:SG   | 11:n:101:GLY:N    | 2.86                     | 0.46              |
| 29:G:42:LEU:H     | 29:G:42:LEU:CD2   | 2.19                     | 0.46              |
| 31:I:99:ASN:O     | 31:I:102:TYR:HB3  | 2.16                     | 0.46              |
| 38:P:32:THR:HA    | 38:P:43:TRP:HA    | 1.96                     | 0.46              |
| 40:R:28:ARG:HA    | 40:R:28:ARG:HD2   | 1.71                     | 0.46              |
| 42:T:71:ARG:HA    | 42:T:71:ARG:HD2   | 1.77                     | 0.46              |
| 44:V:7:LEU:HD21   | 44:V:24:ILE:HG12  | 1.97                     | 0.46              |
| 50:3:1293:C:H2'   | 50:3:1294:G:C8    | 2.51                     | 0.46              |
| 51:1:92:U:H2'     | 51:1:93:G:H5'     | 1.97                     | 0.46              |
| 51:1:226:A:H2'    | 51:1:227:A:O4'    | 2.15                     | 0.46              |
| 51:1:570:G:H4'    | 51:1:983:A:C2     | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:1:609:A:H2'    | 51:1:610:C:O4'    | 2.15                     | 0.46              |
| 51:1:657:U:H2'    | 51:1:658:U:C6     | 2.51                     | 0.46              |
| 51:1:2346:A:H5'   | 51:1:2383:G:HI'   | 1.98                     | 0.46              |
| 51:1:2704:C:H2'   | 51:1:2705:A:O4'   | 2.16                     | 0.46              |
| 52:2:114:C:H2'    | 52:2:115:A:C8     | 2.51                     | 0.46              |
| 3:d:48:THR:CG2    | 3:d:51:GLU:HG3    | 2.45                     | 0.46              |
| 10:m:8:LYS:HG3    | 51:1:869:G:O2'    | 2.16                     | 0.46              |
| 18:u:5:ARG:HG3    | 18:u:93:ARG:NH2   | 2.31                     | 0.46              |
| 19:v:44:HIS:NE2   | 19:v:85:LYS:HB2   | 2.30                     | 0.46              |
| 28:F:16:ILE:CD1   | 28:F:25:VAL:HG22  | 2.45                     | 0.46              |
| 30:H:5:HIS:CD2    | 41:S:88:MET:HB3   | 2.51                     | 0.46              |
| 30:H:168:ARG:NH1  | 50:3:1107:C:H4'   | 2.30                     | 0.46              |
| 32:J:53:ARG:HG2   | 32:J:53:ARG:NH1   | 2.31                     | 0.46              |
| 34:L:94:ARG:HA    | 34:L:97:ALA:HB3   | 1.98                     | 0.46              |
| 35:M:113:ARG:HG2  | 35:M:113:ARG:HH11 | 1.81                     | 0.46              |
| 42:T:6:ALA:HA     | 42:T:9:LYS:HE2    | 1.98                     | 0.46              |
| 42:T:74:VAL:HG12  | 42:T:78:THR:HG23  | 1.98                     | 0.46              |
| 49:a:26:ALA:HB3   | 49:a:224:VAL:HG12 | 1.98                     | 0.46              |
| 49:a:164:ARG:O    | 51:1:2122:U:O2'   | 2.34                     | 0.46              |
| 49:a:216:THR:HG23 | 49:a:221:GLY:HA2  | 1.98                     | 0.46              |
| 50:3:415:A:H2'    | 50:3:416:G:O4'    | 2.16                     | 0.46              |
| 50:3:692:U:H2'    | 50:3:694:A:OP2    | 2.16                     | 0.46              |
| 50:3:864:A:H2'    | 50:3:865:A:C8     | 2.51                     | 0.46              |
| 51:1:1431:A:H2'   | 51:1:1432:G:C8    | 2.51                     | 0.46              |
| 51:1:1571:A:H2'   | 51:1:1572:A:H8    | 1.79                     | 0.46              |
| 55:8:327:VAL:C    | 55:8:328:LEU:HD12 | 2.41                     | 0.46              |
| 2:c:42:ASN:OD1    | 51:1:2784:U:H4'   | 2.15                     | 0.45              |
| 3:d:176:ASP:OD2   | 3:d:178:VAL:HG23  | 2.17                     | 0.45              |
| 5:f:86:LEU:HD12   | 5:f:163:TYR:HA    | 1.98                     | 0.45              |
| 29:G:112:ARG:HG2  | 29:G:112:ARG:HH11 | 1.79                     | 0.45              |
| 30:H:24:ASN:OD1   | 30:H:26:LYS:HB2   | 2.16                     | 0.45              |
| 30:H:99:GLN:HG3   | 30:H:99:GLN:O     | 2.15                     | 0.45              |
| 33:K:20:GLY:O     | 33:K:24:ARG:HG3   | 2.16                     | 0.45              |
| 34:L:47:GLU:C     | 34:L:51:GLN:HG2   | 2.42                     | 0.45              |
| 36:N:74:GLN:O     | 36:N:78:ILE:HG13  | 2.15                     | 0.45              |
| 37:O:10:LEU:HB3   | 37:O:98:VAL:HG22  | 1.98                     | 0.45              |
| 39:Q:35:ARG:N     | 39:Q:75:GLU:OE1   | 2.49                     | 0.45              |
| 41:S:92:ILE:HB    | 41:S:95:LEU:HD12  | 1.98                     | 0.45              |
| 44:V:61:ARG:HB3   | 44:V:61:ARG:CZ    | 2.46                     | 0.45              |
| 50:3:128:G:O2'    | 50:3:129:A:H5'    | 2.16                     | 0.45              |
| 50:3:191:G:H2'    | 50:3:192:A:C8     | 2.51                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 50:3:695:A:H2'   | 50:3:696:A:C8     | 2.51                     | 0.45              |
| 50:3:1256:A:N7   | 50:3:1278:G:H1'   | 2.31                     | 0.45              |
| 51:1:633:A:H1'   | 51:1:2403:C:H4'   | 1.98                     | 0.45              |
| 51:1:704:G:H2'   | 51:1:726:G:H22    | 1.81                     | 0.45              |
| 1:b:135:PRO:HG2  | 1:b:138:SER:OG    | 2.15                     | 0.45              |
| 1:b:225:ASN:HB2  | 1:b:228:ASP:OD2   | 2.16                     | 0.45              |
| 3:d:143:LEU:HD22 | 3:d:146:VAL:HG11  | 1.98                     | 0.45              |
| 7:j:49:ASP:OD2   | 7:j:118:MET:HB3   | 2.16                     | 0.45              |
| 10:m:108:VAL:HB  | 10:m:112:LEU:HD23 | 1.98                     | 0.45              |
| 14:q:80:ASN:HB2  | 51:1:1151:A:O2'   | 2.16                     | 0.45              |
| 16:s:25:ARG:HH11 | 16:s:25:ARG:HG3   | 1.81                     | 0.45              |
| 29:G:46:VAL:N    | 29:G:47:PRO:HD2   | 2.31                     | 0.45              |
| 32:J:151:MET:SD  | 32:J:155:LYS:HE2  | 2.56                     | 0.45              |
| 34:L:90:VAL:HG13 | 34:L:95:ARG:CG    | 2.31                     | 0.45              |
| 39:Q:120:ARG:HD3 | 50:3:37:U:H5''    | 1.98                     | 0.45              |
| 39:Q:120:ARG:HA  | 39:Q:121:PRO:HD3  | 1.76                     | 0.45              |
| 45:W:33:THR:HG22 | 45:W:37:LYS:N     | 2.26                     | 0.45              |
| 47:Y:66:ILE:CD1  | 47:Y:70:LYS:HZ2   | 2.23                     | 0.45              |
| 49:a:215:SER:OG  | 49:a:216:THR:N    | 2.46                     | 0.45              |
| 50:3:195:A:H1'   | 50:3:222:C:O2'    | 2.16                     | 0.45              |
| 50:3:225:C:C2'   | 50:3:226:G:H5''   | 2.46                     | 0.45              |
| 50:3:668:G:H2'   | 50:3:669:G:C8     | 2.51                     | 0.45              |
| 51:1:202:U:H2'   | 51:1:203:A:O4'    | 2.15                     | 0.45              |
| 51:1:254:G:C2'   | 51:1:255:A:H5''   | 2.46                     | 0.45              |
| 51:1:768:G:N2    | 51:1:1379:U:H1'   | 2.30                     | 0.45              |
| 51:1:796:C:H2'   | 51:1:797:G:H8     | 1.81                     | 0.45              |
| 51:1:1028:A:H2'  | 51:1:1029:A:C8    | 2.50                     | 0.45              |
| 51:1:1424:G:H2'  | 51:1:1425:G:O4'   | 2.15                     | 0.45              |
| 51:1:2298:A:H2'  | 51:1:2299:U:H5'   | 1.98                     | 0.45              |
| 51:1:2504:U:C2'  | 51:1:2505:G:H5''  | 2.47                     | 0.45              |
| 51:1:2585:U:OP1  | 55:8:249:ALA:HB2  | 2.17                     | 0.45              |
| 54:4:21:A:H2'    | 55:8:214:HIS:HD2  | 1.81                     | 0.45              |
| 1:b:132:ARG:NH1  | 1:b:133:ASN:OD1   | 2.50                     | 0.45              |
| 2:c:48:ILE:HG23  | 2:c:84:LEU:HD21   | 1.97                     | 0.45              |
| 3:d:163:ASN:HB2  | 51:1:322:A:OP2    | 2.16                     | 0.45              |
| 5:f:41:GLU:HB2   | 5:f:54:ARG:HE     | 1.81                     | 0.45              |
| 8:k:41:ILE:HD11  | 8:k:86:LEU:CD2    | 2.46                     | 0.45              |
| 17:t:73:ARG:HD2  | 51:1:456:C:C2     | 2.51                     | 0.45              |
| 20:w:14:ALA:HB1  | 51:1:2271:G:OP1   | 2.16                     | 0.45              |
| 30:H:20:THR:HG22 | 37:O:94:ALA:O     | 2.16                     | 0.45              |
| 34:L:35:LYS:HA   | 34:L:38:ALA:HB3   | 1.97                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 49:a:7:ARG:HD3   | 51:1:2128:G:H5'   | 1.97                     | 0.45              |
| 50:3:70:U:H4'    | 50:3:71:A:C8      | 2.52                     | 0.45              |
| 50:3:889:A:O3'   | 50:3:890:G:H4'    | 2.17                     | 0.45              |
| 50:3:977:A:H3'   | 50:3:977:A:N3     | 2.32                     | 0.45              |
| 50:3:1443:C:H2'  | 50:3:1444:U:C6    | 2.51                     | 0.45              |
| 52:2:28:C:H2'    | 52:2:29:A:C8      | 2.52                     | 0.45              |
| 55:8:22:ARG:HH21 | 55:8:67:VAL:HA    | 1.81                     | 0.45              |
| 55:8:153:LEU:HA  | 55:8:163:THR:HG21 | 1.97                     | 0.45              |
| 3:d:48:THR:HG22  | 3:d:51:GLU:CG     | 2.41                     | 0.45              |
| 3:d:138:LEU:HD22 | 3:d:143:LEU:HD11  | 1.99                     | 0.45              |
| 5:f:109:SER:HB3  | 51:1:2667:C:N3    | 2.31                     | 0.45              |
| 6:g:115:VAL:HG23 | 6:g:115:VAL:O     | 2.16                     | 0.45              |
| 14:q:60:TRP:O    | 14:q:64:ILE:HG13  | 2.16                     | 0.45              |
| 27:E:4:LYS:HD2   | 51:1:254:G:O6     | 2.17                     | 0.45              |
| 29:G:56:LEU:HD21 | 29:G:220:VAL:HB   | 1.98                     | 0.45              |
| 32:J:149:PRO:HA  | 32:J:152:VAL:HG22 | 1.98                     | 0.45              |
| 35:M:17:GLN:O    | 35:M:20:ASN:ND2   | 2.49                     | 0.45              |
| 49:a:201:PRO:HG2 | 49:a:204:ALA:HB2  | 1.97                     | 0.45              |
| 50:3:113:G:H1'   | 50:3:354:G:C5'    | 2.45                     | 0.45              |
| 50:3:287:U:H2'   | 50:3:288:A:C8     | 2.51                     | 0.45              |
| 50:3:921:U:C5'   | 50:3:1082:A:H5'   | 2.47                     | 0.45              |
| 50:3:948:C:H5'   | 50:3:1306:A:O2'   | 2.16                     | 0.45              |
| 50:3:1354:U:H2'  | 50:3:1355:G:H8    | 1.81                     | 0.45              |
| 51:1:1287:A:C2   | 51:1:1649:G:H4'   | 2.50                     | 0.45              |
| 51:1:1858:A:N6   | 51:1:1884:G:H1'   | 2.31                     | 0.45              |
| 51:1:1917:U:C2'  | 51:1:1918:A:H5'   | 2.46                     | 0.45              |
| 1:b:159:THR:O    | 1:b:194:VAL:HG12  | 2.16                     | 0.45              |
| 1:b:262:THR:HG21 | 51:1:1800:C:P     | 2.57                     | 0.45              |
| 7:j:69:ARG:HA    | 7:j:89:PHE:CD2    | 2.50                     | 0.45              |
| 13:p:50:ARG:NH2  | 51:1:2683:C:H5''  | 2.31                     | 0.45              |
| 23:z:48:ASN:HA   | 23:z:51:SER:OG    | 2.17                     | 0.45              |
| 30:H:21:TRP:HB3  | 30:H:58:ARG:HB3   | 1.98                     | 0.45              |
| 31:I:124:VAL:C   | 31:I:126:GLY:H    | 2.24                     | 0.45              |
| 35:M:48:PHE:O    | 35:M:49:LYS:HD2   | 2.16                     | 0.45              |
| 36:N:53:LEU:HD12 | 36:N:53:LEU:N     | 2.30                     | 0.45              |
| 37:O:92:LEU:C    | 37:O:92:LEU:HD12  | 2.41                     | 0.45              |
| 40:R:5:GLY:O     | 40:R:6:ILE:HD13   | 2.17                     | 0.45              |
| 40:R:36:ALA:HB1  | 40:R:54:THR:HG23  | 1.98                     | 0.45              |
| 48:Z:35:GLU:HG3  | 48:Z:36:PHE:H     | 1.82                     | 0.45              |
| 50:3:67:C:H2'    | 50:3:68:G:C8      | 2.51                     | 0.45              |
| 50:3:1339:A:H2'  | 50:3:1340:A:H5'   | 1.98                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 50:3:1539:C:O2'  | 50:3:1540:U:H5'   | 2.16                     | 0.45              |
| 51:1:366:C:H2'   | 51:1:367:G:C5'    | 2.46                     | 0.45              |
| 51:1:366:C:H2'   | 51:1:367:G:H5''   | 1.98                     | 0.45              |
| 51:1:1979:U:O2'  | 51:1:1980:G:H5'   | 2.16                     | 0.45              |
| 2:c:55:LYS:HG2   | 2:c:56:LYS:N      | 2.32                     | 0.45              |
| 6:g:135:HIS:HB3  | 6:g:138:VAL:HG12  | 1.99                     | 0.45              |
| 9:l:4:ASN:O      | 51:1:1243:C:H1'   | 2.17                     | 0.45              |
| 10:m:64:TRP:HB2  | 10:m:104:GLU:HB2  | 1.98                     | 0.45              |
| 17:t:55:VAL:HA   | 17:t:87:LEU:HA    | 1.98                     | 0.45              |
| 18:u:73:ASN:OD1  | 18:u:75:ALA:HB3   | 2.16                     | 0.45              |
| 21:x:2:ARG:O     | 21:x:11:PRO:HD3   | 2.17                     | 0.45              |
| 31:l:100:VAL:O   | 31:l:104:MET:HG2  | 2.16                     | 0.45              |
| 32:J:44:ARG:HA   | 32:J:72:ASN:HA    | 1.98                     | 0.45              |
| 40:R:18:LEU:O    | 40:R:24:VAL:HG13  | 2.16                     | 0.45              |
| 50:3:225:C:H2'   | 50:3:226:G:H5''   | 1.99                     | 0.45              |
| 50:3:428:G:H4'   | 50:3:429:U:O5'    | 2.17                     | 0.45              |
| 50:3:760:G:H2'   | 50:3:761:G:H5'    | 1.99                     | 0.45              |
| 51:1:862:G:H2'   | 51:1:863:A:O4'    | 2.16                     | 0.45              |
| 51:1:1991:U:H2'  | 51:1:1992:G:C5'   | 2.46                     | 0.45              |
| 51:1:2254:C:H2'  | 51:1:2255:G:H8    | 1.80                     | 0.45              |
| 55:8:189:TYR:CE1 | 55:8:224:PRO:HD3  | 2.51                     | 0.45              |
| 1:b:7:PRO:O      | 51:1:1695:G:H1'   | 2.17                     | 0.45              |
| 2:c:45:TYR:HB2   | 2:c:83:ARG:HH11   | 1.82                     | 0.45              |
| 2:c:110:THR:HG21 | 2:c:169:ARG:HE    | 1.82                     | 0.45              |
| 3:d:111:GLU:OE2  | 3:d:115:GLN:HB2   | 2.17                     | 0.45              |
| 3:d:126:VAL:H    | 3:d:157:LEU:HD11  | 1.81                     | 0.45              |
| 7:j:136:GLN:N    | 7:j:137:PRO:HD3   | 2.32                     | 0.45              |
| 9:l:122:VAL:HG21 | 9:l:135:ILE:HD13  | 1.98                     | 0.45              |
| 15:r:21:ARG:HG3  | 15:r:93:PHE:CD2   | 2.52                     | 0.45              |
| 16:s:13:SER:OG   | 16:s:16:LYS:HG3   | 2.16                     | 0.45              |
| 18:u:13:LEU:HD11 | 18:u:70:ALA:HB2   | 1.97                     | 0.45              |
| 19:v:48:MET:HE3  | 19:v:51:GLN:HB3   | 1.97                     | 0.45              |
| 26:D:43:THR:O    | 26:D:44:VAL:C     | 2.59                     | 0.45              |
| 30:H:69:THR:OG1  | 30:H:70:ALA:N     | 2.49                     | 0.45              |
| 30:H:186:SER:O   | 30:H:197:VAL:HG22 | 2.16                     | 0.45              |
| 32:J:105:ILE:O   | 32:J:105:ILE:HG13 | 2.17                     | 0.45              |
| 39:Q:81:ILE:CG2  | 39:Q:94:TYR:HB3   | 2.47                     | 0.45              |
| 46:X:54:ARG:HG2  | 46:X:54:ARG:NH1   | 2.31                     | 0.45              |
| 46:X:62:THR:H    | 46:X:65:MET:HG3   | 1.81                     | 0.45              |
| 50:3:17:U:H2'    | 50:3:18:C:C6      | 2.52                     | 0.45              |
| 50:3:167:A:C2'   | 50:3:168:G:H5''   | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 50:3:181:A:H61   | 50:3:194:C:H2'   | 1.82                     | 0.45              |
| 50:3:256:U:H2'   | 50:3:257:G:C8    | 2.52                     | 0.45              |
| 50:3:318:G:H2'   | 50:3:319:G:C8    | 2.51                     | 0.45              |
| 50:3:392:C:H2'   | 50:3:393:A:C8    | 2.52                     | 0.45              |
| 50:3:1262:C:H2'  | 50:3:1263:C:O4'  | 2.16                     | 0.45              |
| 50:3:1273:C:H2'  | 50:3:1274:A:H5'  | 1.98                     | 0.45              |
| 51:1:75:G:H2'    | 51:1:75:G:N3     | 2.31                     | 0.45              |
| 51:1:490:C:O2'   | 51:1:491:G:P     | 2.75                     | 0.45              |
| 51:1:2064:C:H2'  | 51:1:2065:C:C6   | 2.52                     | 0.45              |
| 51:1:2105:U:H2'  | 51:1:2106:U:C5'  | 2.47                     | 0.45              |
| 51:1:2730:C:H2'  | 51:1:2731:G:H8   | 1.82                     | 0.45              |
| 1:b:49:THR:OG1   | 1:b:50:THR:N     | 2.50                     | 0.45              |
| 1:b:74:PRO:HD2   | 1:b:96:LYS:HG3   | 1.97                     | 0.45              |
| 4:e:149:ARG:N    | 4:e:149:ARG:HD2  | 2.32                     | 0.45              |
| 5:f:14:VAL:HG13  | 5:f:27:GLY:HA2   | 1.99                     | 0.45              |
| 6:g:122:LEU:HD23 | 6:g:124:THR:O    | 2.17                     | 0.45              |
| 12:o:74:VAL:O    | 12:o:78:VAL:HG23 | 2.17                     | 0.45              |
| 15:r:38:VAL:O    | 15:r:38:VAL:HG13 | 2.16                     | 0.45              |
| 18:u:58:VAL:HG12 | 18:u:59:GLU:N    | 2.31                     | 0.45              |
| 18:u:82:VAL:HG11 | 18:u:93:ARG:HB3  | 1.98                     | 0.45              |
| 29:G:34:ARG:CZ   | 50:3:847:G:H4'   | 2.46                     | 0.45              |
| 35:M:3:GLN:NE2   | 50:3:878:A:H1'   | 2.32                     | 0.45              |
| 40:R:78:ARG:O    | 40:R:82:LEU:N    | 2.45                     | 0.45              |
| 42:T:21:THR:HA   | 42:T:26:VAL:HG11 | 1.99                     | 0.45              |
| 46:X:35:ARG:HD3  | 50:3:1221:G:H5'  | 1.99                     | 0.45              |
| 49:a:5:THR:H     | 49:a:8:MET:HE3   | 1.82                     | 0.45              |
| 50:3:59:A:H5''   | 50:3:387:U:H5''  | 1.98                     | 0.45              |
| 51:1:616:A:H2'   | 51:1:617:G:O4'   | 2.17                     | 0.45              |
| 51:1:1084:A:H2'  | 51:1:1105:U:O2'  | 2.17                     | 0.45              |
| 51:1:1278:C:H2'  | 51:1:1279:G:C8   | 2.52                     | 0.45              |
| 51:1:1932:A:H2'  | 51:1:1933:G:O4'  | 2.17                     | 0.45              |
| 51:1:2259:U:H1'  | 51:1:2427:C:H2'  | 1.98                     | 0.45              |
| 52:2:62:C:H2'    | 52:2:63:C:C6     | 2.52                     | 0.45              |
| 55:8:142:GLN:HB3 | 55:8:175:GLY:HA3 | 1.99                     | 0.45              |
| 1:b:152:GLN:HG3  | 51:1:1818:U:C4   | 2.51                     | 0.45              |
| 2:c:129:THR:HG22 | 2:c:130:GLN:O    | 2.17                     | 0.45              |
| 4:e:176:PHE:CD1  | 4:e:176:PHE:N    | 2.85                     | 0.45              |
| 5:f:86:LEU:HB3   | 5:f:130:ILE:CG2  | 2.47                     | 0.45              |
| 10:m:17:ASN:OD1  | 10:m:95:LEU:HB3  | 2.16                     | 0.45              |
| 11:n:84:GLY:N    | 11:n:85:PRO:HD2  | 2.32                     | 0.45              |
| 19:v:34:LYS:HD2  | 19:v:34:LYS:N    | 2.32                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:B:27:LEU:HD12  | 24:B:36:LYS:HB3   | 1.98                     | 0.45              |
| 29:G:42:LEU:O     | 29:G:46:VAL:HG23  | 2.17                     | 0.45              |
| 29:G:213:LEU:C    | 29:G:213:LEU:HD12 | 2.42                     | 0.45              |
| 32:J:13:LYS:N     | 32:J:37:VAL:O     | 2.50                     | 0.45              |
| 39:Q:43:LYS:HB2   | 39:Q:44:PRO:CD    | 2.47                     | 0.45              |
| 41:S:73:LEU:O     | 41:S:77:GLY:N     | 2.50                     | 0.45              |
| 50:3:694:A:H2     | 50:3:788:U:H5'    | 1.82                     | 0.45              |
| 50:3:829:G:H2'    | 50:3:830:G:H8     | 1.81                     | 0.45              |
| 50:3:1405:G:O2'   | 50:3:1406:U:H5'   | 2.17                     | 0.45              |
| 50:3:1444:U:H2'   | 50:3:1445:U:O4'   | 2.17                     | 0.45              |
| 51:1:420:C:O2'    | 51:1:421:C:H5'    | 2.17                     | 0.45              |
| 51:1:1801:A:O2'   | 51:1:1802:A:H5''  | 2.17                     | 0.45              |
| 52:2:42:C:O2'     | 52:2:43:C:H5'     | 2.17                     | 0.45              |
| 1:b:30:ALA:HB3    | 1:b:31:PRO:HD3    | 1.98                     | 0.45              |
| 1:b:32:LEU:C      | 1:b:33:LEU:HD12   | 2.42                     | 0.45              |
| 1:b:181:ARG:HG3   | 1:b:181:ARG:NH1   | 2.32                     | 0.45              |
| 2:c:209:ALA:HB3   | 51:1:2733:A:H2    | 1.82                     | 0.45              |
| 3:d:147:LEU:HD13  | 3:d:183:PHE:CE2   | 2.52                     | 0.45              |
| 4:e:88:VAL:HA     | 52:2:42:C:O2      | 2.17                     | 0.45              |
| 8:k:71:ARG:HH22   | 8:k:105:ARG:HB2   | 1.81                     | 0.45              |
| 9:l:48:ARG:HH11   | 51:1:666:A:H4'    | 1.82                     | 0.45              |
| 15:r:38:VAL:O     | 15:r:53:PHE:HA    | 2.17                     | 0.45              |
| 16:s:53:SER:O     | 16:s:57:ASN:ND2   | 2.50                     | 0.45              |
| 18:u:44:HIS:CB    | 51:1:482:A:H4'    | 2.47                     | 0.45              |
| 19:v:2:PHE:HB3    | 19:v:50:MET:HE2   | 1.98                     | 0.45              |
| 30:H:85:LYS:O     | 30:H:85:LYS:HD3   | 2.17                     | 0.45              |
| 30:H:190:THR:HG23 | 30:H:192:TYR:H    | 1.81                     | 0.45              |
| 36:N:62:LEU:HD22  | 36:N:62:LEU:N     | 2.32                     | 0.45              |
| 36:N:113:LYS:HA   | 36:N:120:ALA:HB2  | 1.98                     | 0.45              |
| 37:O:13:PHE:HA    | 37:O:69:THR:HA    | 1.98                     | 0.45              |
| 42:T:38:LEU:HD21  | 50:3:741:G:H5'    | 1.99                     | 0.45              |
| 43:U:41:PRO:HB2   | 50:3:450:G:H4'    | 1.98                     | 0.45              |
| 46:X:3:SER:OG     | 50:3:1319:A:H3'   | 2.17                     | 0.45              |
| 47:Y:85:LEU:HD12  | 47:Y:86:ALA:N     | 2.31                     | 0.45              |
| 48:Z:64:ALA:C     | 48:Z:66:ARG:H     | 2.24                     | 0.45              |
| 49:a:190:GLU:O    | 49:a:194:VAL:HG23 | 2.17                     | 0.45              |
| 50:3:665:A:O4'    | 50:3:733:G:H1'    | 2.17                     | 0.45              |
| 50:3:774:G:H2'    | 50:3:775:G:H5'    | 1.99                     | 0.45              |
| 50:3:1195:C:H5''  | 50:3:1196:A:OP2   | 2.17                     | 0.45              |
| 50:3:1270:G:H4'   | 50:3:1313:U:O2'   | 2.17                     | 0.45              |
| 51:1:307:G:N2     | 51:1:309:A:H3'    | 2.32                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 51:1:594:U:H2'   | 51:1:595:C:C6    | 2.52                     | 0.45              |
| 51:1:1063:G:H5'' | 51:1:1064:C:H6   | 1.82                     | 0.45              |
| 51:1:1900:A:H1'  | 51:1:1970:A:H2'  | 1.98                     | 0.45              |
| 51:1:2307:G:H4'  | 51:1:2311:A:C6   | 2.52                     | 0.45              |
| 51:1:2543:G:H2'  | 51:1:2544:G:C8   | 2.52                     | 0.45              |
| 1:b:44:ASN:ND2   | 51:1:1370:C:H4'  | 2.32                     | 0.44              |
| 1:b:62:ARG:NE    | 1:b:84:PRO:HD2   | 2.33                     | 0.44              |
| 2:c:124:ARG:HA   | 2:c:165:MET:SD   | 2.57                     | 0.44              |
| 5:f:69:ALA:CB    | 51:1:2747:G:H5'' | 2.47                     | 0.44              |
| 7:j:8:PRO:HG3    | 7:j:48:VAL:CG1   | 2.47                     | 0.44              |
| 10:m:71:LYS:HB3  | 10:m:93:VAL:O    | 2.18                     | 0.44              |
| 13:p:31:VAL:HG22 | 13:p:32:VAL:H    | 1.82                     | 0.44              |
| 21:x:62:GLY:HA3  | 21:x:65:THR:HG23 | 2.00                     | 0.44              |
| 27:E:4:LYS:HE2   | 51:1:242:G:C5    | 2.52                     | 0.44              |
| 36:N:26:LYS:C    | 36:N:27:ILE:HD12 | 2.41                     | 0.44              |
| 37:O:24:GLU:O    | 37:O:28:THR:HG23 | 2.18                     | 0.44              |
| 43:U:3:THR:HG22  | 43:U:4:ILE:N     | 2.32                     | 0.44              |
| 50:3:393:A:O2'   | 50:3:394:G:H5'   | 2.17                     | 0.44              |
| 50:3:539:A:H2'   | 50:3:540:G:C8    | 2.52                     | 0.44              |
| 50:3:952:U:H2'   | 50:3:953:G:H8    | 1.82                     | 0.44              |
| 51:1:532:A:H2'   | 51:1:532:A:N3    | 2.32                     | 0.44              |
| 51:1:720:U:H2'   | 51:1:721:A:H8    | 1.82                     | 0.44              |
| 51:1:1259:G:H2'  | 51:1:1260:A:C8   | 2.51                     | 0.44              |
| 51:1:2475:C:H42  | 51:1:2529:G:H22  | 1.64                     | 0.44              |
| 51:1:2774:C:H2'  | 51:1:2775:G:O4'  | 2.17                     | 0.44              |
| 52:2:32:U:H2'    | 52:2:33:G:C8     | 2.52                     | 0.44              |
| 1:b:263:ASP:OD1  | 1:b:263:ASP:N    | 2.50                     | 0.44              |
| 3:d:5:LEU:O      | 3:d:9:GLN:NE2    | 2.50                     | 0.44              |
| 4:e:30:VAL:HA    | 4:e:157:THR:HG22 | 1.98                     | 0.44              |
| 4:e:87:LYS:HZ3   | 51:1:2313:C:H4'  | 1.82                     | 0.44              |
| 5:f:39:ALA:O     | 5:f:54:ARG:N     | 2.47                     | 0.44              |
| 5:f:51:PHE:CZ    | 5:f:68:ARG:HA    | 2.52                     | 0.44              |
| 16:s:29:VAL:HG12 | 16:s:55:ILE:HD11 | 2.00                     | 0.44              |
| 17:t:39:THR:HG23 | 17:t:42:GLU:HB2  | 1.97                     | 0.44              |
| 20:w:19:VAL:HG12 | 20:w:20:LYS:N    | 2.32                     | 0.44              |
| 21:x:31:ASN:HB2  | 51:1:2230:G:H1'  | 1.99                     | 0.44              |
| 21:x:70:LEU:HD13 | 21:x:77:TYR:HB3  | 1.99                     | 0.44              |
| 28:F:2:LYS:HB2   | 28:F:35:GLN:HB3  | 1.99                     | 0.44              |
| 33:K:47:LEU:HD13 | 33:K:51:ILE:HG13 | 1.99                     | 0.44              |
| 36:N:10:ARG:O    | 36:N:105:ARG:NH2 | 2.51                     | 0.44              |
| 38:P:33:ILE:CD1  | 38:P:73:VAL:HG11 | 2.44                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 40:R:16:ILE:HA    | 40:R:19:THR:HG22 | 2.00                     | 0.44              |
| 48:Z:22:CYS:SG    | 48:Z:23:GLU:N    | 2.90                     | 0.44              |
| 50:3:255:G:H2'    | 50:3:256:U:C6    | 2.51                     | 0.44              |
| 51:1:1599:U:H2'   | 51:1:1600:C:C6   | 2.52                     | 0.44              |
| 51:1:1683:U:H2'   | 51:1:1684:G:C8   | 2.52                     | 0.44              |
| 51:1:2195:U:H2'   | 51:1:2196:C:C6   | 2.52                     | 0.44              |
| 51:1:2345:G:N3    | 51:1:2381:A:H2'  | 2.32                     | 0.44              |
| 55:8:49:GLU:HB3   | 55:8:52:ARG:HB2  | 1.99                     | 0.44              |
| 55:8:265:HIS:ND1  | 55:8:267:PRO:HD2 | 2.32                     | 0.44              |
| 1:b:52:HIS:CE1    | 1:b:218:THR:HB   | 2.53                     | 0.44              |
| 3:d:117:ARG:HH22  | 9:l:2:ARG:HB2    | 1.83                     | 0.44              |
| 4:e:169:LEU:O     | 4:e:173:ASP:N    | 2.50                     | 0.44              |
| 6:g:61:VAL:O      | 6:g:65:ALA:N     | 2.50                     | 0.44              |
| 15:r:5:PHE:HA     | 15:r:39:LEU:H    | 1.83                     | 0.44              |
| 17:t:11:LEU:HD22  | 22:y:26:PHE:HE1  | 1.82                     | 0.44              |
| 19:v:12:GLN:CD    | 19:v:12:GLN:N    | 2.76                     | 0.44              |
| 20:w:21:ARG:HD2   | 20:w:25:GLU:CD   | 2.42                     | 0.44              |
| 20:w:29:ALA:N     | 20:w:60:ASP:OD1  | 2.51                     | 0.44              |
| 21:x:18:SER:HB2   | 51:1:2080:A:C5'  | 2.48                     | 0.44              |
| 29:G:27:LYS:H     | 29:G:28:PRO:CD   | 2.29                     | 0.44              |
| 29:G:49:PHE:CZ    | 29:G:53:LEU:HD11 | 2.52                     | 0.44              |
| 30:H:180:ASP:OD2  | 30:H:204:GLY:HA3 | 2.17                     | 0.44              |
| 31:I:50:TYR:CD2   | 50:3:508:U:H4'   | 2.52                     | 0.44              |
| 38:P:29:THR:HG21  | 38:P:91:GLY:HA3  | 1.99                     | 0.44              |
| 38:P:118:ASN:HD22 | 50:3:718:A:H5'   | 1.82                     | 0.44              |
| 41:S:60:ARG:NH2   | 50:3:977:A:OP1   | 2.50                     | 0.44              |
| 43:U:60:TRP:HB3   | 43:U:65:ALA:HB2  | 1.97                     | 0.44              |
| 48:Z:64:ALA:O     | 48:Z:66:ARG:N    | 2.50                     | 0.44              |
| 51:1:807:U:H5'    | 51:1:2445:G:H4'  | 1.99                     | 0.44              |
| 51:1:1196:C:H2'   | 51:1:1197:G:C8   | 2.52                     | 0.44              |
| 51:1:1666:G:C2'   | 51:1:1667:G:H5'  | 2.47                     | 0.44              |
| 51:1:1909:C:H2'   | 51:1:1910:G:H8   | 1.81                     | 0.44              |
| 51:1:1909:C:H2'   | 51:1:1910:G:C8   | 2.52                     | 0.44              |
| 51:1:1921:G:O2'   | 51:1:1922:G:H5'  | 2.17                     | 0.44              |
| 51:1:2600:A:C2'   | 51:1:2601:C:H5'  | 2.47                     | 0.44              |
| 52:2:66:A:H5''    | 52:2:67:G:OP1    | 2.16                     | 0.44              |
| 2:c:34:VAL:HB     | 2:c:93:GLY:H     | 1.81                     | 0.44              |
| 3:d:155:GLU:OE2   | 3:d:159:LEU:HG   | 2.17                     | 0.44              |
| 4:e:3:LEU:HD23    | 4:e:99:PHE:CD2   | 2.53                     | 0.44              |
| 6:g:6:LEU:HD11    | 6:g:37:VAL:HG23  | 1.99                     | 0.44              |
| 8:k:31:ARG:N      | 8:k:31:ARG:HD3   | 2.32                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:l:124:GLY:H     | 9:l:144:GLU:HB2   | 1.83                     | 0.44              |
| 16:s:1:MET:H1     | 16:s:110:ARG:HH22 | 1.65                     | 0.44              |
| 18:u:10:VAL:HG13  | 18:u:70:ALA:O     | 2.17                     | 0.44              |
| 29:G:62:ARG:HG2   | 29:G:62:ARG:HH11  | 1.82                     | 0.44              |
| 31:I:101:VAL:HG23 | 31:I:113:ALA:HB1  | 2.00                     | 0.44              |
| 32:J:92:ARG:HH11  | 32:J:92:ARG:HG3   | 1.82                     | 0.44              |
| 36:N:49:GLN:N     | 36:N:50:PRO:HD2   | 2.33                     | 0.44              |
| 37:O:53:ILE:HG21  | 37:O:63:ASP:OD2   | 2.18                     | 0.44              |
| 47:Y:44:ALA:C     | 47:Y:48:LYS:HG2   | 2.41                     | 0.44              |
| 50:3:70:U:H5''    | 50:3:71:A:OP1     | 2.17                     | 0.44              |
| 50:3:514:C:H2'    | 50:3:515:G:C8     | 2.52                     | 0.44              |
| 50:3:1066:C:O2'   | 50:3:1067:A:H5'   | 2.18                     | 0.44              |
| 51:1:832:U:H2'    | 51:1:833:A:C8     | 2.52                     | 0.44              |
| 51:1:1796:U:H2'   | 51:1:1797:G:C8    | 2.52                     | 0.44              |
| 55:8:67:VAL:O     | 55:8:71:ASP:N     | 2.49                     | 0.44              |
| 1:b:97:ASP:O      | 51:1:1500:G:N2    | 2.51                     | 0.44              |
| 6:g:72:ILE:HG23   | 6:g:108:VAL:CG2   | 2.47                     | 0.44              |
| 17:t:13:ALA:HB1   | 22:y:33:ALA:CB    | 2.47                     | 0.44              |
| 30:H:180:ASP:HB2  | 30:H:204:GLY:H    | 1.82                     | 0.44              |
| 39:Q:66:ILE:HA    | 39:Q:96:THR:CG2   | 2.47                     | 0.44              |
| 41:S:12:ARG:HH21  | 50:3:980:C:H4'    | 1.83                     | 0.44              |
| 43:U:67:ILE:CG2   | 43:U:71:VAL:HG23  | 2.46                     | 0.44              |
| 46:X:49:ALA:HB1   | 46:X:56:HIS:HB3   | 2.00                     | 0.44              |
| 47:Y:4:LYS:HD3    | 47:Y:4:LYS:N      | 2.33                     | 0.44              |
| 50:3:45:G:H5''    | 50:3:307:C:O2'    | 2.18                     | 0.44              |
| 50:3:396:C:C3'    | 50:3:397:A:H5''   | 2.48                     | 0.44              |
| 50:3:418:C:H2'    | 50:3:419:C:C6     | 2.52                     | 0.44              |
| 50:3:664:G:H22    | 50:3:741:G:H1     | 1.65                     | 0.44              |
| 51:1:329:G:O4'    | 51:1:477:A:H1'    | 2.17                     | 0.44              |
| 51:1:595:C:H2'    | 51:1:596:U:C6     | 2.53                     | 0.44              |
| 51:1:942:G:H2'    | 51:1:943:A:O4'    | 2.17                     | 0.44              |
| 51:1:991:C:H5'    | 51:1:1185:G:H2'   | 1.99                     | 0.44              |
| 51:1:1340:U:H4'   | 51:1:1394:U:O2'   | 2.17                     | 0.44              |
| 51:1:1505:A:H2'   | 51:1:1506:U:C6    | 2.52                     | 0.44              |
| 51:1:1670:C:H2'   | 51:1:1671:U:H5'   | 1.99                     | 0.44              |
| 51:1:2105:U:H3    | 51:1:2184:A:H61   | 1.65                     | 0.44              |
| 55:8:28:ASP:O     | 55:8:32:GLU:HG3   | 2.18                     | 0.44              |
| 2:c:56:LYS:HB2    | 2:c:59:ARG:CB     | 2.43                     | 0.44              |
| 2:c:157:LYS:HA    | 51:1:2619:C:H5''  | 1.99                     | 0.44              |
| 3:d:118:LEU:HD23  | 3:d:118:LEU:C     | 2.42                     | 0.44              |
| 4:e:4:HIS:O       | 4:e:7:TYR:HB3     | 2.16                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:f:23:ILE:HG21   | 5:f:71:LEU:HD11   | 2.00                     | 0.44              |
| 5:f:140:ILE:HA    | 5:f:143:VAL:HG12  | 1.99                     | 0.44              |
| 12:o:25:ARG:HB2   | 12:o:40:ILE:CG2   | 2.48                     | 0.44              |
| 13:p:4:ILE:HG22   | 13:p:8:GLU:HG3    | 1.99                     | 0.44              |
| 29:G:29:PHE:HD1   | 29:G:41:ASN:OD1   | 2.00                     | 0.44              |
| 29:G:106:VAL:O    | 29:G:110:ILE:HG12 | 2.17                     | 0.44              |
| 29:G:219:THR:O    | 29:G:222:GLU:HG3  | 2.17                     | 0.44              |
| 30:H:48:LYS:HD3   | 30:H:48:LYS:N     | 2.33                     | 0.44              |
| 30:H:78:LYS:H     | 30:H:81:GLU:HG3   | 1.82                     | 0.44              |
| 31:I:197:HIS:CE1  | 32:J:103:GLY:HA3  | 2.52                     | 0.44              |
| 34:L:110:ARG:HG2  | 34:L:110:ARG:O    | 2.18                     | 0.44              |
| 38:P:34:THR:HG23  | 38:P:35:ASP:O     | 2.18                     | 0.44              |
| 40:R:14:ALA:O     | 40:R:18:LEU:N     | 2.46                     | 0.44              |
| 40:R:28:ARG:N     | 50:3:1329:A:OP1   | 2.46                     | 0.44              |
| 50:3:318:G:H2'    | 50:3:319:G:H8     | 1.82                     | 0.44              |
| 50:3:434:U:H2'    | 50:3:435:A:H8     | 1.82                     | 0.44              |
| 50:3:463:U:H3     | 50:3:469:C:N4     | 2.16                     | 0.44              |
| 50:3:493:A:H2'    | 50:3:494:G:C5     | 2.52                     | 0.44              |
| 50:3:1484:C:H2'   | 50:3:1485:U:C6    | 2.53                     | 0.44              |
| 50:3:1492:A:H2    | 54:4:21:A:H5''    | 1.83                     | 0.44              |
| 51:1:9:G:N2       | 51:1:2629:U:H2'   | 2.32                     | 0.44              |
| 51:1:1972:G:H2'   | 51:1:1973:G:H8    | 1.81                     | 0.44              |
| 55:8:103:LEU:HD23 | 55:8:103:LEU:C    | 2.42                     | 0.44              |
| 55:8:334:LYS:CE   | 55:8:339:GLY:HA2  | 2.47                     | 0.44              |
| 1:b:70:LYS:HD2    | 1:b:99:GLU:OE2    | 2.18                     | 0.44              |
| 2:c:101:PHE:O     | 2:c:104:VAL:HG12  | 2.18                     | 0.44              |
| 4:e:94:ARG:HA     | 4:e:97:GLU:HB3    | 1.98                     | 0.44              |
| 8:k:97:THR:O      | 8:k:118:LEU:HD13  | 2.18                     | 0.44              |
| 8:k:99:ILE:HD12   | 8:k:115:ILE:O     | 2.18                     | 0.44              |
| 11:n:48:VAL:O     | 11:n:52:ILE:HG13  | 2.18                     | 0.44              |
| 14:q:8:ILE:HG23   | 14:q:9:ALA:N      | 2.31                     | 0.44              |
| 14:q:103:VAL:O    | 14:q:106:THR:HG22 | 2.17                     | 0.44              |
| 15:r:21:ARG:HG3   | 15:r:93:PHE:HD2   | 1.83                     | 0.44              |
| 16:s:88:ARG:HG3   | 16:s:94:ASP:CG    | 2.43                     | 0.44              |
| 22:y:21:LEU:HA    | 22:y:25:GLN:HB3   | 1.99                     | 0.44              |
| 23:z:35:VAL:HG22  | 23:z:37:ARG:HH12  | 1.82                     | 0.44              |
| 29:G:101:THR:OG1  | 50:3:1074:G:H5''  | 2.16                     | 0.44              |
| 31:I:28:ASP:OD1   | 31:I:28:ASP:N     | 2.50                     | 0.44              |
| 36:N:78:ILE:O     | 36:N:82:ILE:HG13  | 2.18                     | 0.44              |
| 40:R:16:ILE:HG12  | 50:3:1302:C:C6    | 2.53                     | 0.44              |
| 40:R:93:GLY:HA2   | 40:R:108:ARG:HH12 | 1.83                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 44:V:4:ILE:HG23  | 44:V:4:ILE:O      | 2.18                     | 0.44              |
| 50:3:411:A:OP2   | 50:3:429:U:H5     | 2.00                     | 0.44              |
| 50:3:918:A:H2'   | 50:3:919:A:O4'    | 2.18                     | 0.44              |
| 50:3:1186:G:O2'  | 50:3:1187:G:H5'   | 2.18                     | 0.44              |
| 51:1:345:A:H2    | 51:1:346:A:H62    | 1.65                     | 0.44              |
| 51:1:414:C:H2'   | 51:1:415:A:C8     | 2.53                     | 0.44              |
| 51:1:487:C:H2'   | 51:1:488:G:O4'    | 2.17                     | 0.44              |
| 51:1:704:G:H2'   | 51:1:726:G:N2     | 2.33                     | 0.44              |
| 51:1:826:U:H2'   | 51:1:828:U:O4'    | 2.17                     | 0.44              |
| 51:1:1680:U:C2'  | 51:1:1681:G:H5'   | 2.48                     | 0.44              |
| 55:8:33:ARG:O    | 55:8:37:VAL:N     | 2.45                     | 0.44              |
| 55:8:132:ILE:HB  | 55:8:179:VAL:HG23 | 1.99                     | 0.44              |
| 55:8:324:ARG:HG3 | 55:8:324:ARG:HH11 | 1.82                     | 0.44              |
| 1:b:164:VAL:HG21 | 1:b:180:MET:HE1   | 2.00                     | 0.44              |
| 2:c:123:LYS:NZ   | 51:1:2724:U:H5''  | 2.33                     | 0.44              |
| 4:e:55:ASP:OD1   | 4:e:55:ASP:N      | 2.51                     | 0.44              |
| 5:f:85:LYS:HG3   | 5:f:164:ALA:HB3   | 2.00                     | 0.44              |
| 6:g:9:VAL:CG2    | 6:g:13:GLY:HA3    | 2.44                     | 0.44              |
| 6:g:60:GLU:O     | 6:g:63:ALA:HB3    | 2.17                     | 0.44              |
| 10:m:109:PRO:HG2 | 10:m:112:LEU:HB3  | 2.00                     | 0.44              |
| 13:p:27:VAL:CG1  | 13:p:42:PHE:HB3   | 2.47                     | 0.44              |
| 14:q:36:GLN:NE2  | 51:1:564:C:H1'    | 2.33                     | 0.44              |
| 15:r:91:GLN:NE2  | 51:1:993:G:N3     | 2.66                     | 0.44              |
| 31:I:205:LYS:HB2 | 50:3:8:A:C6       | 2.53                     | 0.44              |
| 39:Q:62:VAL:HG22 | 39:Q:63:THR:N     | 2.33                     | 0.44              |
| 46:X:30:LEU:H    | 46:X:48:ILE:HG22  | 1.83                     | 0.44              |
| 48:Z:39:LYS:HE2  | 50:3:1507:A:H62   | 1.83                     | 0.44              |
| 49:a:24:ASN:CB   | 49:a:186:LYS:HG3  | 2.41                     | 0.44              |
| 49:a:27:ILE:O    | 49:a:30:LEU:HB3   | 2.18                     | 0.44              |
| 50:3:45:G:H2'    | 50:3:46:G:C8      | 2.53                     | 0.44              |
| 50:3:411:A:H1'   | 50:3:413:G:C1'    | 2.47                     | 0.44              |
| 51:1:368:A:H2'   | 51:1:369:U:O4'    | 2.18                     | 0.44              |
| 51:1:372:G:O2'   | 51:1:373:U:H5     | 2.01                     | 0.44              |
| 51:1:1609:A:H1'  | 51:1:1616:A:O4'   | 2.18                     | 0.44              |
| 51:1:1664:A:H2'  | 51:1:1664:A:N3    | 2.32                     | 0.44              |
| 55:8:73:MET:SD   | 55:8:73:MET:C     | 3.01                     | 0.44              |
| 55:8:264:THR:C   | 55:8:291:MET:HE1  | 2.43                     | 0.44              |
| 55:8:337:ARG:NH2 | 55:8:361:LEU:HD11 | 2.32                     | 0.44              |
| 55:8:357:ILE:HA  | 55:8:361:LEU:HB2  | 2.00                     | 0.44              |
| 3:d:5:LEU:O      | 3:d:7:ASP:N       | 2.51                     | 0.44              |
| 4:e:63:LYS:O     | 52:2:42:C:O2'     | 2.33                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:e:87:LYS:NZ     | 51:1:2313:C:H4'   | 2.33                     | 0.44              |
| 5:f:34:ARG:HG3    | 5:f:35:THR:O      | 2.18                     | 0.44              |
| 6:g:31:VAL:N      | 6:g:32:PRO:HD2    | 2.32                     | 0.44              |
| 6:g:134:VAL:HG23  | 6:g:138:VAL:CG1   | 2.44                     | 0.44              |
| 8:k:70:ARG:HG2    | 8:k:76:VAL:CG1    | 2.46                     | 0.44              |
| 14:q:96:ASP:O     | 14:q:99:VAL:HG12  | 2.18                     | 0.44              |
| 18:u:45:GLN:HB3   | 18:u:55:GLY:O     | 2.17                     | 0.44              |
| 18:u:98:ASN:O     | 18:u:100:GLU:N    | 2.51                     | 0.44              |
| 30:H:45:GLU:C     | 30:H:46:LEU:HD12  | 2.43                     | 0.44              |
| 30:H:161:ILE:HG22 | 50:3:1196:A:C2    | 2.52                     | 0.44              |
| 36:N:110:VAL:HG13 | 50:3:1348:U:OP2   | 2.17                     | 0.44              |
| 39:Q:38:THR:HG22  | 39:Q:39:THR:N     | 2.33                     | 0.44              |
| 41:S:98:ALA:HB1   | 41:S:100:TRP:HZ3  | 1.83                     | 0.44              |
| 45:W:37:LYS:HA    | 50:3:719:C:O2     | 2.18                     | 0.44              |
| 49:a:189:LEU:HA   | 49:a:192:LEU:HB3  | 1.99                     | 0.44              |
| 50:3:70:U:H4'     | 50:3:71:A:H8      | 1.83                     | 0.44              |
| 50:3:836:G:H2'    | 50:3:837:U:H5'    | 2.00                     | 0.44              |
| 50:3:1493:A:O2'   | 55:8:136:SER:HA   | 2.18                     | 0.44              |
| 51:1:818:G:O2'    | 51:1:819:A:H5''   | 2.18                     | 0.44              |
| 51:1:1060:U:H4'   | 51:1:1062:G:H5''  | 1.99                     | 0.44              |
| 51:1:2073:C:O2'   | 51:1:2074:U:H5'   | 2.17                     | 0.44              |
| 51:1:2403:C:H2'   | 51:1:2404:U:C6    | 2.53                     | 0.44              |
| 53:5:37:A:H2'     | 53:5:38:A:O4'     | 2.18                     | 0.44              |
| 55:8:52:ARG:HD2   | 55:8:52:ARG:N     | 2.33                     | 0.44              |
| 55:8:294:LYS:O    | 55:8:298:LEU:HG   | 2.18                     | 0.44              |
| 55:8:322:GLN:CD   | 55:8:322:GLN:N    | 2.76                     | 0.44              |
| 2:c:142:VAL:HG22  | 2:c:143:PRO:HD2   | 2.00                     | 0.43              |
| 3:d:27:LEU:HD23   | 3:d:27:LEU:O      | 2.18                     | 0.43              |
| 3:d:148:ILE:HA    | 3:d:187:VAL:CG2   | 2.48                     | 0.43              |
| 6:g:72:ILE:CG2    | 6:g:108:VAL:HG22  | 2.48                     | 0.43              |
| 10:m:2:LEU:HB2    | 10:m:69:PRO:HG2   | 2.00                     | 0.43              |
| 13:p:94:ALA:HB2   | 51:1:2848:G:N7    | 2.33                     | 0.43              |
| 19:v:17:SER:OG    | 19:v:27:PRO:HG3   | 2.18                     | 0.43              |
| 24:B:15:ARG:HG3   | 24:B:15:ARG:HH21  | 1.84                     | 0.43              |
| 28:F:16:ILE:HD12  | 28:F:25:VAL:HG22  | 1.99                     | 0.43              |
| 29:G:173:LYS:O    | 29:G:177:ASN:ND2  | 2.50                     | 0.43              |
| 30:H:123:LEU:HD23 | 30:H:123:LEU:C    | 2.43                     | 0.43              |
| 31:I:56:GLU:OE2   | 31:I:194:ILE:HD12 | 2.18                     | 0.43              |
| 32:J:64:GLU:C     | 32:J:68:ARG:HH12  | 2.26                     | 0.43              |
| 32:J:105:ILE:CG1  | 32:J:123:LEU:HA   | 2.47                     | 0.43              |
| 34:L:91:ARG:NE    | 34:L:91:ARG:HA    | 2.33                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 35:M:14:ARG:HH22 | 50:3:876:C:H4'    | 1.83                     | 0.43              |
| 36:N:68:GLY:HA2  | 50:3:1250:A:H5'   | 2.00                     | 0.43              |
| 36:N:73:GLY:N    | 50:3:1372:U:OP1   | 2.48                     | 0.43              |
| 37:O:11:LYS:NZ   | 37:O:99:GLN:NE2   | 2.66                     | 0.43              |
| 37:O:59:LYS:HD2  | 50:3:972:C:O3'    | 2.18                     | 0.43              |
| 38:P:58:THR:OG1  | 38:P:59:PRO:HD2   | 2.18                     | 0.43              |
| 39:Q:3:VAL:HA    | 39:Q:6:LEU:HD12   | 2.00                     | 0.43              |
| 39:Q:32:VAL:CG2  | 39:Q:55:ARG:HB3   | 2.48                     | 0.43              |
| 43:U:35:ARG:HG3  | 43:U:35:ARG:O     | 2.18                     | 0.43              |
| 44:V:61:ARG:NH1  | 44:V:75:VAL:HG22  | 2.33                     | 0.43              |
| 45:W:26:ALA:O    | 45:W:30:ASN:ND2   | 2.51                     | 0.43              |
| 45:W:48:ALA:HB2  | 50:3:834:U:H5''   | 2.00                     | 0.43              |
| 46:X:20:LYS:HA   | 46:X:23:GLU:OE2   | 2.17                     | 0.43              |
| 48:Z:16:ARG:HD2  | 48:Z:18:PHE:CB    | 2.48                     | 0.43              |
| 50:3:1094:G:N3   | 50:3:1094:G:C2'   | 2.81                     | 0.43              |
| 50:3:1170:A:H2'  | 50:3:1171:A:C5'   | 2.47                     | 0.43              |
| 50:3:1245:C:H2'  | 50:3:1246:A:H8    | 1.83                     | 0.43              |
| 51:1:6:A:H2'     | 51:1:7:G:C8       | 2.53                     | 0.43              |
| 51:1:28:A:H1'    | 51:1:513:A:C2     | 2.53                     | 0.43              |
| 51:1:2655:G:O2'  | 51:1:2656:U:H5    | 2.01                     | 0.43              |
| 53:5:3:C:H2'     | 53:5:4:G:O4'      | 2.18                     | 0.43              |
| 53:5:29:G:O2'    | 53:5:30:G:H5'     | 2.18                     | 0.43              |
| 55:8:75:GLN:O    | 55:8:79:ASP:N     | 2.50                     | 0.43              |
| 55:8:130:LEU:HG  | 55:8:222:VAL:HG22 | 1.99                     | 0.43              |
| 2:c:99:GLU:OE2   | 2:c:182:ALA:HB2   | 2.18                     | 0.43              |
| 4:e:68:LYS:HG2   | 4:e:83:PRO:N      | 2.33                     | 0.43              |
| 6:g:51:ARG:O     | 6:g:55:GLU:HB3    | 2.18                     | 0.43              |
| 7:j:35:ARG:HA    | 7:j:40:HIS:HD2    | 1.83                     | 0.43              |
| 10:m:54:THR:HB   | 10:m:63:ILE:HD11  | 2.00                     | 0.43              |
| 16:s:18:ARG:CZ   | 51:1:518:G:H4'    | 2.48                     | 0.43              |
| 25:C:21:THR:HG23 | 27:E:33:THR:HG22  | 1.99                     | 0.43              |
| 29:G:113:LEU:O   | 29:G:117:GLU:HG2  | 2.17                     | 0.43              |
| 29:G:166:ASP:HB3 | 29:G:190:SER:HA   | 1.99                     | 0.43              |
| 30:H:29:ALA:C    | 41:S:64:ARG:HH22  | 2.25                     | 0.43              |
| 31:I:67:LEU:O    | 31:I:71:PHE:N     | 2.48                     | 0.43              |
| 31:I:137:SER:N   | 31:I:140:ASP:OD2  | 2.51                     | 0.43              |
| 35:M:106:SER:HA  | 50:3:642:A:C6     | 2.53                     | 0.43              |
| 36:N:57:VAL:HG23 | 36:N:58:GLU:N     | 2.30                     | 0.43              |
| 41:S:5:MET:CE    | 50:3:982:U:H3'    | 2.48                     | 0.43              |
| 50:3:1099:G:H2'  | 50:3:1100:C:O4'   | 2.17                     | 0.43              |
| 51:1:1496:A:H1'  | 51:1:1578:U:H4'   | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:1:1557:C:H5''  | 51:1:1559:U:O4    | 2.18                     | 0.43              |
| 51:1:1771:C:H2'   | 51:1:1772:A:C8    | 2.53                     | 0.43              |
| 51:1:2011:U:H2'   | 51:1:2012:G:O4'   | 2.17                     | 0.43              |
| 51:1:2339:C:H2'   | 51:1:2340:A:C8    | 2.53                     | 0.43              |
| 51:1:2583:G:H2'   | 51:1:2584:U:H5'   | 2.00                     | 0.43              |
| 52:2:106:G:H2'    | 52:2:107:G:O4'    | 2.18                     | 0.43              |
| 52:2:117:G:H2'    | 52:2:118:C:O4'    | 2.18                     | 0.43              |
| 53:5:62:C:H2'     | 53:5:63:G:H8      | 1.83                     | 0.43              |
| 1:b:116:GLN:CD    | 1:b:121:ALA:HA    | 2.43                     | 0.43              |
| 3:d:1:MET:SD      | 3:d:16:GLU:HA     | 2.58                     | 0.43              |
| 5:f:156:TYR:CE1   | 51:1:2531:A:H4'   | 2.54                     | 0.43              |
| 10:m:97:GLN:OE1   | 10:m:97:GLN:N     | 2.51                     | 0.43              |
| 12:o:51:ALA:HA    | 12:o:55:GLU:OE2   | 2.18                     | 0.43              |
| 14:q:30:VAL:HB    | 14:q:33:VAL:HG12  | 2.01                     | 0.43              |
| 15:r:28:ALA:O     | 15:r:66:HIS:NE2   | 2.52                     | 0.43              |
| 26:D:21:ARG:O     | 26:D:27:GLY:HA3   | 2.18                     | 0.43              |
| 28:F:36:ARG:O     | 28:F:37:GLN:HB3   | 2.18                     | 0.43              |
| 29:G:169:HIS:O    | 29:G:173:LYS:HG2  | 2.19                     | 0.43              |
| 32:J:105:ILE:HG13 | 32:J:123:LEU:HA   | 2.00                     | 0.43              |
| 33:K:1:MET:HE3    | 33:K:67:PRO:HB3   | 2.00                     | 0.43              |
| 41:S:79:SER:CB    | 41:S:82:LYS:HG2   | 2.42                     | 0.43              |
| 50:3:27:G:H2'     | 50:3:28:A:C8      | 2.53                     | 0.43              |
| 50:3:460:A:H2'    | 50:3:461:A:H8     | 1.84                     | 0.43              |
| 51:1:12:U:O2'     | 51:1:13:A:H5'     | 2.18                     | 0.43              |
| 51:1:277:G:H3'    | 51:1:277:G:N3     | 2.32                     | 0.43              |
| 51:1:987:C:H2'    | 51:1:988:A:O4'    | 2.18                     | 0.43              |
| 51:1:1507:C:O2'   | 51:1:1508:A:H4'   | 2.17                     | 0.43              |
| 7:j:114:LEU:O     | 7:j:118:MET:HG2   | 2.19                     | 0.43              |
| 10:m:27:SER:O     | 10:m:29:GLY:N     | 2.52                     | 0.43              |
| 12:o:51:ALA:HB2   | 12:o:81:ARG:CD    | 2.48                     | 0.43              |
| 25:C:35:LEU:HD11  | 51:1:2344:U:O2'   | 2.17                     | 0.43              |
| 30:H:127:VAL:CG2  | 30:H:128:MET:N    | 2.80                     | 0.43              |
| 32:J:38:VAL:HG12  | 32:J:66:ALA:HB1   | 2.00                     | 0.43              |
| 32:J:108:GLY:H    | 50:3:9:G:H5'      | 1.83                     | 0.43              |
| 33:K:6:ILE:HD13   | 33:K:74:LEU:CD2   | 2.48                     | 0.43              |
| 38:P:124:LYS:HZ3  | 48:Z:33:ARG:C     | 2.26                     | 0.43              |
| 39:Q:29:LYS:O     | 39:Q:80:LEU:HD12  | 2.19                     | 0.43              |
| 40:R:106:ARG:HB3  | 40:R:106:ARG:HH11 | 1.79                     | 0.43              |
| 41:S:45:LEU:HD11  | 46:X:12:LEU:HA    | 1.99                     | 0.43              |
| 49:a:23:ILE:HG23  | 49:a:24:ASN:N     | 2.34                     | 0.43              |
| 50:3:256:U:H2'    | 50:3:257:G:H8     | 1.84                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 51:1:1368:G:H2'   | 51:1:1369:G:H8   | 1.84                     | 0.43              |
| 51:1:2297:A:C2    | 51:1:2321:U:H5   | 2.36                     | 0.43              |
| 1:b:179:GLU:HG2   | 1:b:268:ARG:O    | 2.18                     | 0.43              |
| 2:c:161:MET:HE1   | 51:1:2050:C:H1'  | 2.00                     | 0.43              |
| 5:f:22:VAL:HG12   | 5:f:35:THR:HA    | 2.01                     | 0.43              |
| 8:k:76:VAL:HG22   | 13:p:72:VAL:CG2  | 2.48                     | 0.43              |
| 9:l:19:LEU:HD23   | 51:1:587:C:C2    | 2.54                     | 0.43              |
| 13:p:24:THR:HG23  | 13:p:86:LYS:CB   | 2.36                     | 0.43              |
| 14:q:89:ILE:HG12  | 15:r:39:LEU:CD2  | 2.48                     | 0.43              |
| 25:C:5:ARG:HE     | 25:C:23:THR:HG23 | 1.84                     | 0.43              |
| 29:G:23:ASN:HB3   | 29:G:26:MET:HG2  | 2.00                     | 0.43              |
| 30:H:107:LYS:HD2  | 30:H:109:GLU:HB3 | 2.00                     | 0.43              |
| 30:H:113:LYS:HE2  | 30:H:184:ASN:OD1 | 2.17                     | 0.43              |
| 30:H:139:ASN:O    | 30:H:143:LEU:HB2 | 2.19                     | 0.43              |
| 30:H:196:GLY:HA3  | 50:3:1057:G:O2'  | 2.18                     | 0.43              |
| 31:I:36:ALA:N     | 31:I:37:PRO:CD   | 2.80                     | 0.43              |
| 33:K:79:ARG:HH12  | 50:3:671:G:H4'   | 1.84                     | 0.43              |
| 34:L:117:LEU:O    | 34:L:121:ASN:ND2 | 2.52                     | 0.43              |
| 42:T:67:ASP:O     | 42:T:71:ARG:N    | 2.51                     | 0.43              |
| 50:3:704:A:H2'    | 50:3:705:G:O4'   | 2.18                     | 0.43              |
| 51:1:1561:C:H2'   | 51:1:1562:U:C6   | 2.52                     | 0.43              |
| 51:1:2420:C:O2'   | 51:1:2421:G:H5'  | 2.19                     | 0.43              |
| 51:1:2756:U:H3    | 51:1:2758:A:H62  | 1.64                     | 0.43              |
| 51:1:2860:A:C2'   | 51:1:2861:U:H5'  | 2.48                     | 0.43              |
| 4:e:75:GLY:HA3    | 51:1:2311:A:C4   | 2.54                     | 0.43              |
| 20:w:66:GLU:O     | 20:w:75:PHE:N    | 2.45                     | 0.43              |
| 25:C:36:LYS:HE3   | 51:1:2344:U:OP1  | 2.18                     | 0.43              |
| 26:D:3:ARG:O      | 26:D:6:GLN:NE2   | 2.52                     | 0.43              |
| 33:K:4:TYR:HB3    | 33:K:89:VAL:HG13 | 2.01                     | 0.43              |
| 33:K:14:GLN:HE21  | 33:K:17:GLN:NE2  | 2.16                     | 0.43              |
| 36:N:17:ARG:NH1   | 50:3:1128:C:O2'  | 2.50                     | 0.43              |
| 36:N:47:VAL:HG12  | 36:N:78:ILE:HB   | 2.00                     | 0.43              |
| 36:N:72:SER:OG    | 50:3:1372:U:OP1  | 2.25                     | 0.43              |
| 38:P:40:ALA:HB2   | 50:3:706:A:H2    | 1.83                     | 0.43              |
| 39:Q:113:ARG:HH21 | 39:Q:120:ARG:HD2 | 1.83                     | 0.43              |
| 43:U:35:ARG:HG3   | 43:U:35:ARG:HH11 | 1.84                     | 0.43              |
| 44:V:26:ARG:CZ    | 50:3:237:G:H5''  | 2.49                     | 0.43              |
| 46:X:54:ARG:CZ    | 46:X:55:GLN:HE21 | 2.30                     | 0.43              |
| 50:3:150:U:H2'    | 50:3:151:A:H8    | 1.83                     | 0.43              |
| 50:3:1192:C:H2'   | 50:3:1193:G:O4'  | 2.17                     | 0.43              |
| 50:3:1256:A:H1'   | 50:3:1258:G:C8   | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:3:1521:C:H2'   | 50:3:1522:U:C6    | 2.54                     | 0.43              |
| 51:1:1179:G:C3'   | 51:1:1180:U:H4'   | 2.48                     | 0.43              |
| 51:1:1427:A:H4'   | 51:1:1428:C:H5'   | 1.99                     | 0.43              |
| 51:1:1879:C:H2'   | 51:1:1880:U:C6    | 2.53                     | 0.43              |
| 51:1:2105:U:H2'   | 51:1:2106:U:C4'   | 2.48                     | 0.43              |
| 51:1:2208:C:H2'   | 51:1:2209:G:H8    | 1.80                     | 0.43              |
| 51:1:2308:G:H3'   | 51:1:2309:A:H5'   | 1.99                     | 0.43              |
| 54:4:19:U:O2      | 55:8:138:GLY:HA3  | 2.18                     | 0.43              |
| 20:w:7:ARG:NH2    | 53:5:2:G:H5'      | 2.33                     | 0.43              |
| 29:G:94:ARG:HH12  | 50:3:1103:C:H5'   | 1.84                     | 0.43              |
| 31:I:100:VAL:O    | 31:I:104:MET:N    | 2.51                     | 0.43              |
| 32:J:110:MET:HA   | 32:J:113:VAL:HG12 | 2.00                     | 0.43              |
| 40:R:114:PRO:C    | 50:3:1228:C:H5''  | 2.44                     | 0.43              |
| 47:Y:67:HIS:C     | 47:Y:69:ASN:H     | 2.26                     | 0.43              |
| 48:Z:16:ARG:NH1   | 48:Z:19:LYS:NZ    | 2.67                     | 0.43              |
| 50:3:218:U:H2'    | 50:3:219:U:O4'    | 2.19                     | 0.43              |
| 50:3:219:U:O2'    | 50:3:220:G:H5'    | 2.19                     | 0.43              |
| 50:3:1241:G:H2'   | 50:3:1242:G:C8    | 2.51                     | 0.43              |
| 51:1:210:C:H2'    | 51:1:211:C:C6     | 2.54                     | 0.43              |
| 51:1:372:G:O2'    | 51:1:373:U:C5     | 2.72                     | 0.43              |
| 51:1:395:U:H2'    | 51:1:396:G:C8     | 2.53                     | 0.43              |
| 51:1:962:G:H2'    | 51:1:963:U:C6     | 2.54                     | 0.43              |
| 51:1:1258:U:H2'   | 51:1:1259:G:H8    | 1.84                     | 0.43              |
| 51:1:1447:C:H2'   | 51:1:1448:G:C8    | 2.53                     | 0.43              |
| 51:1:2234:G:H2'   | 51:1:2235:G:O4'   | 2.19                     | 0.43              |
| 51:1:2338:C:H2'   | 51:1:2339:C:C6    | 2.54                     | 0.43              |
| 51:1:2376:A:H2'   | 51:1:2377:A:O4'   | 2.19                     | 0.43              |
| 51:1:2531:A:C2    | 51:1:2659:G:H4'   | 2.53                     | 0.43              |
| 55:8:109:LYS:O    | 55:8:113:LEU:HD13 | 2.18                     | 0.43              |
| 13:p:77:SER:HA    | 13:p:78:PRO:HD3   | 1.90                     | 0.43              |
| 13:p:83:ILE:N     | 13:p:83:ILE:CD1   | 2.80                     | 0.43              |
| 16:s:70:LYS:O     | 16:s:107:VAL:HG23 | 2.19                     | 0.43              |
| 16:s:82:MET:HB2   | 16:s:98:LYS:HB2   | 2.01                     | 0.43              |
| 24:B:2:VAL:CG2    | 24:B:3:GLN:N      | 2.82                     | 0.43              |
| 24:B:31:LYS:HA    | 24:B:31:LYS:HD3   | 1.83                     | 0.43              |
| 28:F:16:ILE:HD13  | 28:F:25:VAL:HG13  | 2.00                     | 0.43              |
| 30:H:123:LEU:HD13 | 30:H:188:ALA:CB   | 2.49                     | 0.43              |
| 31:I:88:ASN:O     | 31:I:92:LEU:HG    | 2.18                     | 0.43              |
| 36:N:77:ALA:O     | 36:N:81:GLY:N     | 2.52                     | 0.43              |
| 38:P:86:LYS:HD2   | 38:P:114:PRO:HD3  | 1.99                     | 0.43              |
| 39:Q:38:THR:HG23  | 39:Q:49:ARG:C     | 2.43                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 39:Q:85:ARG:HA   | 39:Q:93:ARG:HA   | 2.00                     | 0.43              |
| 40:R:14:ALA:HA   | 40:R:17:ALA:HB3  | 2.01                     | 0.43              |
| 41:S:52:ARG:HH22 | 46:X:13:HIS:HD2  | 1.67                     | 0.43              |
| 43:U:10:GLY:O    | 50:3:624:C:H4'   | 2.19                     | 0.43              |
| 45:W:40:PRO:HG2  | 45:W:42:ARG:HG2  | 1.99                     | 0.43              |
| 45:W:52:ARG:HE   | 50:3:664:G:H5'   | 1.83                     | 0.43              |
| 46:X:66:VAL:O    | 46:X:68:HIS:N    | 2.51                     | 0.43              |
| 50:3:118:U:H2'   | 50:3:119:A:H5'   | 2.01                     | 0.43              |
| 50:3:335:C:H2'   | 50:3:336:A:C8    | 2.54                     | 0.43              |
| 50:3:407:U:H2'   | 50:3:408:A:H8    | 1.84                     | 0.43              |
| 51:1:115:C:O2'   | 51:1:116:C:H5'   | 2.19                     | 0.43              |
| 51:1:154:U:H2'   | 51:1:155:A:C8    | 2.54                     | 0.43              |
| 51:1:1739:A:H2'  | 51:1:1740:G:C8   | 2.53                     | 0.43              |
| 51:1:1811:G:H2'  | 51:1:1812:U:C6   | 2.53                     | 0.43              |
| 52:2:42:C:H2'    | 52:2:43:C:O4'    | 2.18                     | 0.43              |
| 55:8:290:GLN:O   | 55:8:294:LYS:HG2 | 2.19                     | 0.43              |
| 1:b:77:VAL:HG11  | 1:b:109:LEU:HD21 | 2.01                     | 0.43              |
| 2:c:173:GLN:HE22 | 2:c:208:LYS:NZ   | 2.16                     | 0.43              |
| 6:g:54:LEU:HD23  | 6:g:54:LEU:C     | 2.44                     | 0.43              |
| 7:j:43:GLU:OE1   | 7:j:43:GLU:N     | 2.45                     | 0.43              |
| 7:j:99:ARG:HA    | 7:j:102:GLU:HG2  | 2.00                     | 0.43              |
| 14:q:36:GLN:HE21 | 51:1:564:C:C1'   | 2.32                     | 0.43              |
| 17:t:28:ASN:ND2  | 17:t:88:LYS:O    | 2.52                     | 0.43              |
| 28:F:18:LYS:HA   | 28:F:23:ILE:HA   | 2.01                     | 0.43              |
| 29:G:94:ARG:HG3  | 50:3:1100:C:C5   | 2.53                     | 0.43              |
| 29:G:220:VAL:O   | 29:G:224:ARG:N   | 2.51                     | 0.43              |
| 33:K:36:ILE:HA   | 33:K:64:VAL:HG23 | 2.00                     | 0.43              |
| 33:K:37:HIS:HB3  | 33:K:97:THR:CG2  | 2.46                     | 0.43              |
| 33:K:56:LYS:HD2  | 33:K:56:LYS:N    | 2.32                     | 0.43              |
| 34:L:102:TRP:HA  | 34:L:105:GLU:OE2 | 2.18                     | 0.43              |
| 35:M:64:TYR:HA   | 35:M:69:ALA:HA   | 2.01                     | 0.43              |
| 47:Y:35:TYR:CD1  | 47:Y:38:ILE:HD12 | 2.54                     | 0.43              |
| 47:Y:36:ALA:O    | 47:Y:39:GLU:HB2  | 2.19                     | 0.43              |
| 50:3:314:C:O2'   | 50:3:315:A:H5'   | 2.18                     | 0.43              |
| 50:3:632:U:H3'   | 50:3:633:G:H5'   | 1.99                     | 0.43              |
| 50:3:1236:A:H2'  | 50:3:1237:C:C6   | 2.54                     | 0.43              |
| 50:3:1306:A:O2'  | 50:3:1307:U:H5'  | 2.19                     | 0.43              |
| 50:3:1391:U:H2'  | 50:3:1392:G:C8   | 2.54                     | 0.43              |
| 51:1:631:A:H2'   | 51:1:632:A:O4'   | 2.19                     | 0.43              |
| 51:1:1848:A:H2'  | 51:1:1849:G:O4'  | 2.18                     | 0.43              |
| 51:1:2554:U:H2'  | 51:1:2555:U:C6   | 2.53                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 51:1:2581:G:H4'   | 51:1:2582:G:H5'  | 2.01                     | 0.43              |
| 51:1:2740:A:H2'   | 51:1:2741:A:C8   | 2.53                     | 0.43              |
| 55:8:33:ARG:HD2   | 55:8:36:GLU:HB2  | 2.00                     | 0.43              |
| 2:c:47:ALA:HB2    | 2:c:83:ARG:HA    | 2.00                     | 0.43              |
| 4:e:109:ARG:HD3   | 4:e:136:ILE:C    | 2.43                     | 0.43              |
| 9:l:48:ARG:HD2    | 27:E:59:ALA:O    | 2.19                     | 0.43              |
| 10:m:57:VAL:O     | 10:m:58:LYS:HB2  | 2.19                     | 0.43              |
| 29:G:65:LYS:HD3   | 29:G:153:MET:HE1 | 2.01                     | 0.43              |
| 33:K:42:TRP:CH2   | 33:K:61:LEU:HD22 | 2.54                     | 0.43              |
| 34:L:31:VAL:HG22  | 34:L:32:ASP:CG   | 2.44                     | 0.43              |
| 34:L:148:LYS:HG2  | 34:L:148:LYS:O   | 2.18                     | 0.43              |
| 41:S:11:LYS:O     | 41:S:15:LEU:HD13 | 2.18                     | 0.43              |
| 42:T:32:THR:CB    | 42:T:84:LEU:HD21 | 2.48                     | 0.43              |
| 46:X:37:SER:O     | 46:X:70:LEU:N    | 2.49                     | 0.43              |
| 50:3:431:A:H2'    | 50:3:432:A:C8    | 2.54                     | 0.43              |
| 50:3:1287:A:H2    | 50:3:1353:G:H1'  | 1.83                     | 0.43              |
| 51:1:118:A:OP2    | 51:1:119:A:H2'   | 2.19                     | 0.43              |
| 51:1:1161:C:H2'   | 51:1:1162:G:C8   | 2.54                     | 0.43              |
| 51:1:1210:G:H5''  | 51:1:1212:G:O4'  | 2.19                     | 0.43              |
| 51:1:1721:G:H21   | 51:1:1722:A:H62  | 1.65                     | 0.43              |
| 51:1:1771:C:H2'   | 51:1:1772:A:H8   | 1.84                     | 0.43              |
| 51:1:1812:U:H2'   | 51:1:1813:G:H8   | 1.84                     | 0.43              |
| 51:1:1851:U:H2'   | 51:1:1852:U:O4'  | 2.19                     | 0.43              |
| 51:1:2065:C:H2'   | 51:1:2066:C:C6   | 2.54                     | 0.43              |
| 51:1:2339:C:H2'   | 51:1:2340:A:H8   | 1.83                     | 0.43              |
| 55:8:11:ILE:HG21  | 55:8:80:VAL:HG11 | 2.01                     | 0.43              |
| 55:8:144:TRP:CZ2  | 55:8:201:LEU:HB2 | 2.53                     | 0.43              |
| 2:c:129:THR:HG23  | 2:c:140:HIS:O    | 2.18                     | 0.42              |
| 5:f:108:PHE:HA    | 51:1:2666:C:N4   | 2.34                     | 0.42              |
| 10:m:64:TRP:HZ3   | 10:m:106:ASP:CB  | 2.32                     | 0.42              |
| 14:q:101:ASP:HB3  | 14:q:104:ALA:HB3 | 2.00                     | 0.42              |
| 18:u:16:LYS:HG2   | 51:1:329:G:N1    | 2.32                     | 0.42              |
| 22:y:47:ARG:HB2   | 22:y:47:ARG:HH21 | 1.84                     | 0.42              |
| 27:E:43:LEU:HD22  | 27:E:43:LEU:N    | 2.34                     | 0.42              |
| 31:I:7:LYS:HE3    | 50:3:408:A:OP2   | 2.19                     | 0.42              |
| 31:I:143:SER:OG   | 31:I:144:ILE:N   | 2.51                     | 0.42              |
| 32:J:133:ILE:HG23 | 32:J:134:ASN:N   | 2.33                     | 0.42              |
| 33:K:22:ILE:HA    | 33:K:25:TYR:HD2  | 1.83                     | 0.42              |
| 33:K:55:HIS:O     | 33:K:56:LYS:C    | 2.62                     | 0.42              |
| 34:L:27:ASN:HB3   | 50:3:1374:A:O2'  | 2.19                     | 0.42              |
| 34:L:59:GLU:O     | 34:L:63:VAL:HG22 | 2.19                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 45:W:48:ALA:CB  | 50:3:834:U:H5''  | 2.49                     | 0.42              |
| 50:3:349:A:O2'  | 50:3:350:G:H5'   | 2.19                     | 0.42              |
| 50:3:1014:A:H2' | 50:3:1015:G:O4'  | 2.19                     | 0.42              |
| 50:3:1123:U:H2' | 50:3:1124:G:C8   | 2.54                     | 0.42              |
| 50:3:1158:C:H2' | 50:3:1159:U:C4'  | 2.46                     | 0.42              |
| 50:3:1225:A:H2' | 50:3:1225:A:N3   | 2.33                     | 0.42              |
| 51:1:181:A:H2'  | 51:1:182:A:C8    | 2.54                     | 0.42              |
| 51:1:549:G:H2'  | 51:1:550:C:C6    | 2.53                     | 0.42              |
| 51:1:1465:G:H4' | 51:1:1527:G:O2'  | 2.18                     | 0.42              |
| 51:1:2024:G:H2' | 51:1:2025:C:C6   | 2.54                     | 0.42              |
| 51:1:2259:U:O2' | 51:1:2427:C:H2'  | 2.18                     | 0.42              |
| 51:1:2698:U:H2' | 51:1:2699:C:C6   | 2.54                     | 0.42              |
| 52:2:105:G:H2'  | 52:2:106:G:O4'   | 2.18                     | 0.42              |
| 2:c:88:GLU:CD   | 2:c:88:GLU:N     | 2.77                     | 0.42              |
| 6:g:116:ARG:C   | 6:g:117:LEU:HD12 | 2.44                     | 0.42              |
| 11:n:40:LYS:HE3 | 51:1:1651:G:OP1  | 2.19                     | 0.42              |
| 15:r:22:LEU:N   | 15:r:22:LEU:HD23 | 2.34                     | 0.42              |
| 16:s:8:ARG:HG2  | 16:s:102:HIS:ND1 | 2.34                     | 0.42              |
| 19:v:80:HIS:CE1 | 19:v:81:PRO:HD2  | 2.54                     | 0.42              |
| 19:v:80:HIS:HE1 | 19:v:82:TYR:CE1  | 2.37                     | 0.42              |
| 29:G:2:THR:HG22 | 29:G:3:VAL:N     | 2.33                     | 0.42              |
| 30:H:39:ARG:HG3 | 30:H:54:ILE:HD11 | 2.02                     | 0.42              |
| 37:O:12:ALA:O   | 37:O:70:HIS:N    | 2.49                     | 0.42              |
| 38:P:61:ALA:O   | 38:P:65:ALA:N    | 2.50                     | 0.42              |
| 43:U:47:GLU:H   | 43:U:47:GLU:CD   | 2.27                     | 0.42              |
| 46:X:31:ARG:HA  | 46:X:49:ALA:HB3  | 2.01                     | 0.42              |
| 50:3:497:G:H2'  | 50:3:498:A:C8    | 2.54                     | 0.42              |
| 50:3:517:G:H4'  | 50:3:519:C:C2    | 2.54                     | 0.42              |
| 50:3:694:A:H2'  | 50:3:695:A:O4'   | 2.19                     | 0.42              |
| 50:3:744:C:H2'  | 50:3:745:G:C8    | 2.55                     | 0.42              |
| 50:3:763:G:H2'  | 50:3:764:C:C6    | 2.54                     | 0.42              |
| 50:3:1513:A:H2' | 50:3:1514:G:H8   | 1.84                     | 0.42              |
| 51:1:360:U:H2'  | 51:1:361:G:O4'   | 2.19                     | 0.42              |
| 51:1:1447:C:H2' | 51:1:1448:G:H8   | 1.83                     | 0.42              |
| 51:1:2579:C:O2' | 51:1:2580:U:H5'  | 2.19                     | 0.42              |
| 52:2:3:C:C3'    | 52:2:4:C:C5'     | 2.96                     | 0.42              |
| 3:d:3:LEU:HB3   | 3:d:120:VAL:HG11 | 2.01                     | 0.42              |
| 4:e:30:VAL:HA   | 4:e:157:THR:HA   | 2.00                     | 0.42              |
| 4:e:116:LEU:CD1 | 51:1:2304:G:H4'  | 2.48                     | 0.42              |
| 5:f:163:TYR:HB2 | 5:f:166:GLU:CD   | 2.44                     | 0.42              |
| 11:n:47:VAL:C   | 11:n:50:PRO:HD2  | 2.44                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:o:51:ALA:HB2  | 12:o:81:ARG:NE    | 2.33                     | 0.42              |
| 13:p:30:TRP:CE3  | 13:p:30:TRP:HA    | 2.53                     | 0.42              |
| 26:D:24:THR:HG23 | 26:D:27:GLY:N     | 2.23                     | 0.42              |
| 29:G:160:LEU:HG  | 29:G:180:ILE:CD1  | 2.49                     | 0.42              |
| 30:H:37:LYS:O    | 30:H:40:GLN:HG3   | 2.20                     | 0.42              |
| 34:L:104:VAL:O   | 34:L:108:ARG:HG2  | 2.18                     | 0.42              |
| 35:M:15:ASN:HD21 | 50:3:874:G:H22    | 1.67                     | 0.42              |
| 35:M:113:ARG:NH1 | 35:M:117:GLN:OE1  | 2.53                     | 0.42              |
| 37:O:42:LEU:HA   | 37:O:43:PRO:HD2   | 1.82                     | 0.42              |
| 37:O:76:ILE:N    | 37:O:76:ILE:CD1   | 2.83                     | 0.42              |
| 39:Q:120:ARG:HG3 | 39:Q:120:ARG:HH11 | 1.85                     | 0.42              |
| 40:R:15:VAL:HG11 | 40:R:40:GLU:CD    | 2.44                     | 0.42              |
| 41:S:42:ASN:O    | 41:S:46:LYS:N     | 2.52                     | 0.42              |
| 41:S:63:CYS:O    | 41:S:67:GLY:N     | 2.52                     | 0.42              |
| 50:3:865:A:H2'   | 50:3:866:C:C6     | 2.54                     | 0.42              |
| 50:3:1002:G:H2'  | 50:3:1003:G:O4'   | 2.19                     | 0.42              |
| 50:3:1273:C:C2'  | 50:3:1274:A:H5'   | 2.49                     | 0.42              |
| 50:3:1388:C:H2'  | 50:3:1389:C:C6    | 2.54                     | 0.42              |
| 51:1:277:G:H5'   | 51:1:278:A:C5'    | 2.46                     | 0.42              |
| 51:1:634:C:H2'   | 51:1:635:C:C6     | 2.54                     | 0.42              |
| 51:1:1448:G:H2'  | 51:1:1449:G:H8    | 1.83                     | 0.42              |
| 52:2:29:A:H2'    | 52:2:30:C:C6      | 2.55                     | 0.42              |
| 52:2:30:C:H2'    | 52:2:31:C:C5'     | 2.49                     | 0.42              |
| 54:4:8:A:H2'     | 54:4:9:G:H8       | 1.84                     | 0.42              |
| 55:8:36:GLU:O    | 55:8:39:ALA:HB3   | 2.19                     | 0.42              |
| 4:e:104:THR:C    | 4:e:108:PRO:HG3   | 2.45                     | 0.42              |
| 12:o:87:ILE:O    | 12:o:88:LYS:HD3   | 2.19                     | 0.42              |
| 18:u:43:LYS:HA   | 51:1:481:G:OP2    | 2.19                     | 0.42              |
| 20:w:36:GLN:HE21 | 20:w:53:HIS:HB3   | 1.84                     | 0.42              |
| 29:G:96:LEU:HD23 | 29:G:96:LEU:C     | 2.44                     | 0.42              |
| 30:H:131:ARG:O   | 30:H:135:ARG:HB2  | 2.20                     | 0.42              |
| 32:J:12:GLU:HG3  | 32:J:38:VAL:CG2   | 2.50                     | 0.42              |
| 32:J:23:THR:HG22 | 32:J:28:ARG:HG2   | 2.01                     | 0.42              |
| 32:J:137:ARG:CZ  | 50:3:1078:U:H4'   | 2.49                     | 0.42              |
| 32:J:160:VAL:HA  | 32:J:163:ILE:CD1  | 2.50                     | 0.42              |
| 41:S:74:ARG:HG3  | 50:3:1359:C:OP2   | 2.19                     | 0.42              |
| 45:W:27:THR:HA   | 45:W:30:ASN:ND2   | 2.34                     | 0.42              |
| 50:3:818:G:H3'   | 50:3:819:A:C5'    | 2.49                     | 0.42              |
| 51:1:296:U:H2'   | 51:1:297:G:H8     | 1.84                     | 0.42              |
| 51:1:327:G:O2'   | 51:1:328:U:H5'    | 2.20                     | 0.42              |
| 51:1:662:G:O2'   | 51:1:663:G:H5'    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:1:856:G:H2'    | 51:1:857:G:C8     | 2.54                     | 0.42              |
| 51:1:995:C:H6     | 51:1:995:C:H5'    | 1.85                     | 0.42              |
| 51:1:1060:U:O4'   | 51:1:1062:G:H5''  | 2.19                     | 0.42              |
| 51:1:1153:C:H2'   | 51:1:1154:G:O4'   | 2.19                     | 0.42              |
| 51:1:1190:G:H2'   | 51:1:1191:G:C8    | 2.54                     | 0.42              |
| 51:1:1386:C:H2'   | 51:1:1387:A:C8    | 2.55                     | 0.42              |
| 51:1:2024:G:OP2   | 51:1:2034:U:H4'   | 2.19                     | 0.42              |
| 51:1:2220:U:H2'   | 51:1:2221:G:C8    | 2.54                     | 0.42              |
| 51:1:2508:G:OP1   | 55:8:245:ARG:NH2  | 2.52                     | 0.42              |
| 52:2:88:C:H5''    | 52:2:89:U:OP1     | 2.19                     | 0.42              |
| 2:c:40:LEU:HD12   | 2:c:40:LEU:N      | 2.28                     | 0.42              |
| 3:d:31:VAL:HG13   | 3:d:32:VAL:N      | 2.34                     | 0.42              |
| 3:d:117:ARG:NH2   | 9:l:2:ARG:HB2     | 2.35                     | 0.42              |
| 4:e:134:GLN:NE2   | 4:e:135:ILE:HG23  | 2.34                     | 0.42              |
| 5:f:174:LYS:HD3   | 51:1:2531:A:OP1   | 2.20                     | 0.42              |
| 7:j:5:THR:HG21    | 51:1:537:G:C5'    | 2.49                     | 0.42              |
| 7:j:113:PRO:HD2   | 51:1:558:U:OP1    | 2.18                     | 0.42              |
| 9:l:92:LEU:HG     | 9:l:93:ASN:H      | 1.85                     | 0.42              |
| 15:r:1:MET:SD     | 15:r:1:MET:C      | 3.03                     | 0.42              |
| 22:y:58:ASN:HD22  | 51:1:112:U:H5'    | 1.85                     | 0.42              |
| 29:G:46:VAL:HA    | 29:G:49:PHE:HB3   | 2.02                     | 0.42              |
| 29:G:128:LEU:N    | 29:G:128:LEU:HD23 | 2.34                     | 0.42              |
| 29:G:128:LEU:HD23 | 29:G:128:LEU:H    | 1.85                     | 0.42              |
| 31:I:115:GLN:NE2  | 50:3:406:G:H1'    | 2.34                     | 0.42              |
| 31:I:151:GLN:OE1  | 31:I:151:GLN:HA   | 2.19                     | 0.42              |
| 31:I:153:ARG:HH11 | 31:I:153:ARG:HG3  | 1.84                     | 0.42              |
| 32:J:10:LEU:HG    | 32:J:11:GLN:N     | 2.35                     | 0.42              |
| 33:K:42:TRP:HE1   | 33:K:101:PRO:HG3  | 1.84                     | 0.42              |
| 35:M:49:LYS:O     | 35:M:58:LEU:HA    | 2.20                     | 0.42              |
| 38:P:118:ASN:O    | 50:3:716:A:N3     | 2.53                     | 0.42              |
| 39:Q:65:TYR:O     | 39:Q:96:THR:HG22  | 2.20                     | 0.42              |
| 43:U:5:ARG:HD2    | 50:3:376:G:O3'    | 2.20                     | 0.42              |
| 44:V:46:HIS:N     | 44:V:72:TRP:O     | 2.41                     | 0.42              |
| 48:Z:66:ARG:HD2   | 48:Z:66:ARG:HA    | 1.72                     | 0.42              |
| 50:3:920:U:H2'    | 50:3:921:U:C6     | 2.54                     | 0.42              |
| 50:3:1144:G:O2'   | 50:3:1145:A:H5'   | 2.19                     | 0.42              |
| 50:3:1258:G:H2'   | 50:3:1259:C:C6    | 2.55                     | 0.42              |
| 51:1:910:A:H2'    | 51:1:911:A:C8     | 2.55                     | 0.42              |
| 2:c:133:THR:HG23  | 2:c:134:HIS:CD2   | 2.54                     | 0.42              |
| 3:d:98:LYS:O      | 3:d:102:ARG:HD3   | 2.20                     | 0.42              |
| 3:d:148:ILE:O     | 3:d:170:ARG:N     | 2.52                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 17:t:15:HIS:HB3   | 17:t:31:VAL:HG12 | 2.01                     | 0.42              |
| 17:t:57:VAL:HG22  | 17:t:58:VAL:N    | 2.34                     | 0.42              |
| 20:w:67:VAL:O     | 20:w:67:VAL:HG13 | 2.19                     | 0.42              |
| 31:I:58:GLN:HE21  | 31:I:62:ARG:CD   | 2.32                     | 0.42              |
| 33:K:54:LEU:HD12  | 33:K:54:LEU:HA   | 1.89                     | 0.42              |
| 36:N:31:GLN:HB2   | 36:N:32:ARG:NH2  | 2.35                     | 0.42              |
| 37:O:8:ILE:HG13   | 37:O:98:VAL:CG1  | 2.49                     | 0.42              |
| 40:R:95:PRO:N     | 40:R:108:ARG:HG2 | 2.35                     | 0.42              |
| 47:Y:2:ASN:N      | 50:3:332:G:OP2   | 2.52                     | 0.42              |
| 48:Z:35:GLU:CG    | 48:Z:36:PHE:N    | 2.83                     | 0.42              |
| 48:Z:36:PHE:C     | 48:Z:38:GLU:H    | 2.28                     | 0.42              |
| 50:3:405:U:H3'    | 50:3:406:G:C5'   | 2.42                     | 0.42              |
| 50:3:1052:U:O4    | 50:3:1200:C:H2'  | 2.19                     | 0.42              |
| 50:3:1280:A:HO2'  | 50:3:1281:C:H5'  | 1.85                     | 0.42              |
| 50:3:1496:C:H2'   | 50:3:1497:G:O4'  | 2.19                     | 0.42              |
| 51:1:626:A:H3'    | 51:1:627:A:C5'   | 2.50                     | 0.42              |
| 51:1:1440:U:H2'   | 51:1:1441:G:C8   | 2.55                     | 0.42              |
| 51:1:2224:G:H4'   | 51:1:2226:C:O2   | 2.18                     | 0.42              |
| 51:1:2788:C:H2'   | 51:1:2789:C:C6   | 2.55                     | 0.42              |
| 51:1:2811:G:O2'   | 51:1:2812:G:H5'  | 2.20                     | 0.42              |
| 1:b:219:VAL:HG11  | 51:1:782:A:N7    | 2.34                     | 0.42              |
| 3:d:97:ASN:ND2    | 3:d:100:MET:SD   | 2.91                     | 0.42              |
| 3:d:122:GLU:HG2   | 3:d:123:LYS:N    | 2.33                     | 0.42              |
| 3:d:122:GLU:HB2   | 3:d:123:LYS:HD2  | 2.01                     | 0.42              |
| 4:e:148:VAL:HG23  | 4:e:148:VAL:O    | 2.20                     | 0.42              |
| 11:n:83:LEU:HD22  | 11:n:83:LEU:N    | 2.35                     | 0.42              |
| 15:r:10:LYS:HD2   | 15:r:10:LYS:N    | 2.34                     | 0.42              |
| 17:t:33:LYS:HG2   | 17:t:80:TRP:CZ3  | 2.55                     | 0.42              |
| 18:u:10:VAL:HG13  | 18:u:70:ALA:C    | 2.45                     | 0.42              |
| 26:D:39:ARG:NH1   | 51:1:467:G:N7    | 2.66                     | 0.42              |
| 27:E:5:THR:HG23   | 27:E:63:TYR:HD2  | 1.84                     | 0.42              |
| 27:E:14:LYS:HG2   | 27:E:22:LYS:HE2  | 2.00                     | 0.42              |
| 29:G:182:VAL:HB   | 29:G:195:VAL:HA  | 2.02                     | 0.42              |
| 29:G:186:VAL:HG12 | 29:G:187:ASP:O   | 2.20                     | 0.42              |
| 32:J:23:THR:HA    | 32:J:28:ARG:HA   | 2.01                     | 0.42              |
| 35:M:112:ASP:O    | 35:M:116:ARG:HG3 | 2.19                     | 0.42              |
| 40:R:101:THR:OG1  | 50:3:1225:A:H5'  | 2.20                     | 0.42              |
| 41:S:45:LEU:HD12  | 41:S:48:GLN:NE2  | 2.35                     | 0.42              |
| 49:a:197:LYS:HA   | 49:a:200:LYS:HE3 | 2.01                     | 0.42              |
| 51:1:191:A:H2'    | 51:1:192:C:C6    | 2.54                     | 0.42              |
| 51:1:351:C:H2'    | 51:1:352:A:C8    | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:1:2143:C:H2'   | 51:1:2144:G:C5'   | 2.47                     | 0.42              |
| 51:1:2314:A:O2'   | 51:1:2315:G:H8    | 2.03                     | 0.42              |
| 51:1:2786:U:O2'   | 51:1:2787:C:H5'   | 2.19                     | 0.42              |
| 55:8:117:ARG:HD3  | 55:8:117:ARG:C    | 2.45                     | 0.42              |
| 55:8:193:ARG:HG2  | 55:8:193:ARG:HH11 | 1.83                     | 0.42              |
| 55:8:343:ARG:C    | 55:8:344:ASN:HD22 | 2.27                     | 0.42              |
| 1:b:132:ARG:HH21  | 6:g:123:ARG:HG3   | 1.85                     | 0.42              |
| 2:c:115:GLY:O     | 51:1:2822:G:OP2   | 2.38                     | 0.42              |
| 7:j:4:PHE:O       | 14:q:63:ARG:NH2   | 2.51                     | 0.42              |
| 7:j:4:PHE:CD2     | 14:q:99:VAL:HG21  | 2.55                     | 0.42              |
| 12:o:106:LEU:C    | 12:o:106:LEU:HD23 | 2.45                     | 0.42              |
| 12:o:106:LEU:HD23 | 12:o:106:LEU:O    | 2.20                     | 0.42              |
| 17:t:66:LYS:H     | 17:t:77:ARG:HB2   | 1.85                     | 0.42              |
| 32:J:158:LYS:N    | 32:J:158:LYS:HD2  | 2.34                     | 0.42              |
| 36:N:8:THR:O      | 36:N:81:GLY:HA2   | 2.19                     | 0.42              |
| 40:R:24:VAL:HG13  | 40:R:24:VAL:O     | 2.20                     | 0.42              |
| 42:T:64:LYS:HA    | 42:T:67:ASP:OD2   | 2.20                     | 0.42              |
| 43:U:33:ILE:H     | 43:U:33:ILE:CD1   | 2.33                     | 0.42              |
| 49:a:192:LEU:HD23 | 49:a:196:LEU:HD23 | 2.02                     | 0.42              |
| 49:a:217:THR:O    | 51:1:2124:G:N2    | 2.53                     | 0.42              |
| 50:3:89:U:O2'     | 50:3:90:C:H5'     | 2.19                     | 0.42              |
| 50:3:205:A:H2'    | 50:3:206:C:O4'    | 2.20                     | 0.42              |
| 51:1:366:C:C2'    | 51:1:367:G:H5''   | 2.49                     | 0.42              |
| 51:1:803:U:O2'    | 51:1:804:A:H5'    | 2.20                     | 0.42              |
| 51:1:839:U:H2'    | 51:1:840:C:C6     | 2.55                     | 0.42              |
| 51:1:1010:A:N3    | 51:1:1153:C:H1'   | 2.35                     | 0.42              |
| 51:1:1508:A:O2'   | 51:1:1509:A:H4'   | 2.19                     | 0.42              |
| 52:2:40:U:H1'     | 52:2:43:C:H5      | 1.85                     | 0.42              |
| 55:8:201:LEU:HD12 | 55:8:326:TYR:HB2  | 2.01                     | 0.42              |
| 1:b:75:ALA:HB1    | 1:b:93:VAL:HG21   | 2.01                     | 0.42              |
| 10:m:59:ARG:HA    | 10:m:59:ARG:NE    | 2.35                     | 0.42              |
| 10:m:69:PRO:HA    | 10:m:94:ALA:HB2   | 2.01                     | 0.42              |
| 12:o:102:ARG:N    | 52:2:49:C:OP1     | 2.46                     | 0.42              |
| 13:p:108:ARG:C    | 13:p:109:ILE:HD12 | 2.45                     | 0.42              |
| 23:z:45:GLY:HA3   | 51:1:851:C:O2'    | 2.20                     | 0.42              |
| 29:G:66:ILE:HA    | 29:G:159:ALA:HB3  | 2.01                     | 0.42              |
| 31:I:155:LYS:O    | 31:I:158:LEU:HG   | 2.19                     | 0.42              |
| 32:J:24:VAL:N     | 32:J:27:GLY:O     | 2.47                     | 0.42              |
| 35:M:79:ARG:HB3   | 50:3:878:A:OP1    | 2.20                     | 0.42              |
| 37:O:70:HIS:HB3   | 37:O:72:ARG:HH12  | 1.84                     | 0.42              |
| 38:P:24:ALA:N     | 38:P:86:LYS:O     | 2.46                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 38:P:28:ASN:ND2  | 38:P:56:LYS:NZ   | 2.68                     | 0.42              |
| 44:V:13:SER:HB3  | 44:V:21:VAL:CG2  | 2.50                     | 0.42              |
| 47:Y:28:ARG:HH11 | 47:Y:28:ARG:HG3  | 1.84                     | 0.42              |
| 50:3:335:C:H2'   | 50:3:336:A:H8    | 1.85                     | 0.42              |
| 50:3:425:G:O2'   | 50:3:426:U:H5'   | 2.20                     | 0.42              |
| 50:3:1261:A:H1'  | 50:3:1275:A:N1   | 2.34                     | 0.42              |
| 51:1:437:U:H2'   | 51:1:438:G:C8    | 2.54                     | 0.42              |
| 51:1:687:C:H2'   | 51:1:688:U:O4'   | 2.19                     | 0.42              |
| 51:1:1873:G:H2'  | 51:1:1874:C:C6   | 2.55                     | 0.42              |
| 51:1:2162:G:H5'' | 51:1:2171:A:N7   | 2.35                     | 0.42              |
| 55:8:11:ILE:HD13 | 55:8:80:VAL:HG11 | 2.01                     | 0.42              |
| 6:g:5:LEU:HB2    | 6:g:17:ASP:H     | 1.85                     | 0.42              |
| 8:k:78:ARG:HH22  | 13:p:100:ARG:NH1 | 2.18                     | 0.42              |
| 9:l:124:GLY:C    | 9:l:125:LEU:HD12 | 2.45                     | 0.42              |
| 13:p:26:GLU:N    | 13:p:84:SER:O    | 2.46                     | 0.42              |
| 14:q:67:ALA:HB1  | 14:q:105:PHE:CE2 | 2.54                     | 0.42              |
| 26:D:44:VAL:HG13 | 26:D:44:VAL:O    | 2.19                     | 0.42              |
| 30:H:29:ALA:HB1  | 41:S:64:ARG:HH22 | 1.85                     | 0.42              |
| 31:I:75:TYR:HA   | 31:I:89:LEU:HD21 | 2.01                     | 0.42              |
| 32:J:92:ARG:HG3  | 32:J:92:ARG:NH1  | 2.35                     | 0.42              |
| 36:N:105:ARG:HD2 | 36:N:105:ARG:O   | 2.19                     | 0.42              |
| 36:N:125:GLN:HG3 | 50:3:1232:U:OP1  | 2.20                     | 0.42              |
| 46:X:5:LYS:HG2   | 50:3:1313:U:OP1  | 2.20                     | 0.42              |
| 50:3:348:G:O2'   | 50:3:349:A:H5'   | 2.20                     | 0.42              |
| 50:3:917:G:H2'   | 50:3:918:A:C8    | 2.55                     | 0.42              |
| 50:3:1427:C:H2'  | 50:3:1428:A:C8   | 2.55                     | 0.42              |
| 50:3:1481:U:H2'  | 50:3:1482:G:C8   | 2.55                     | 0.42              |
| 51:1:297:G:H2'   | 51:1:298:G:O4'   | 2.20                     | 0.42              |
| 51:1:679:C:H2'   | 51:1:680:C:C6    | 2.55                     | 0.42              |
| 51:1:768:G:H22   | 51:1:1379:U:H1'  | 1.85                     | 0.42              |
| 51:1:1421:G:H2'  | 51:1:1422:G:C8   | 2.55                     | 0.42              |
| 51:1:2236:U:H2'  | 51:1:2237:G:O4'  | 2.19                     | 0.42              |
| 51:1:2508:G:N1   | 51:1:2580:U:H5   | 2.15                     | 0.42              |
| 51:1:2741:A:H2'  | 51:1:2742:G:O4'  | 2.19                     | 0.42              |
| 53:5:3:C:O2'     | 53:5:4:G:H5'     | 2.20                     | 0.42              |
| 1:b:61:TYR:HE1   | 51:1:1817:G:OP1  | 2.03                     | 0.41              |
| 2:c:184:ARG:HG2  | 2:c:184:ARG:HH21 | 1.84                     | 0.41              |
| 6:g:11:ASN:ND2   | 51:1:2095:A:H5'  | 2.34                     | 0.41              |
| 7:j:35:ARG:HG2   | 7:j:35:ARG:HH11  | 1.85                     | 0.41              |
| 7:j:45:THR:HA    | 7:j:46:PRO:HD2   | 1.89                     | 0.41              |
| 11:n:118:ARG:NH1 | 24:B:55:ALA:HB3  | 2.35                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:q:2:ARG:HA    | 51:1:1248:G:O2'   | 2.20                     | 0.41              |
| 21:x:27:ARG:NH1  | 51:1:1808:A:C6    | 2.88                     | 0.41              |
| 24:B:54:ILE:HG23 | 24:B:56:LYS:H     | 1.85                     | 0.41              |
| 28:F:37:GLN:O    | 51:1:1124:G:O2'   | 2.37                     | 0.41              |
| 30:H:110:LEU:HB3 | 30:H:203:LYS:HE3  | 2.02                     | 0.41              |
| 31:I:9:LYS:HE2   | 50:3:542:G:OP1    | 2.20                     | 0.41              |
| 34:L:101:ARG:CZ  | 50:3:939:G:H4'    | 2.50                     | 0.41              |
| 36:N:46:VAL:HG13 | 36:N:47:VAL:N     | 2.35                     | 0.41              |
| 38:P:85:VAL:HG13 | 38:P:111:ASP:HA   | 2.01                     | 0.41              |
| 44:V:16:MET:O    | 44:V:19:SER:HB2   | 2.20                     | 0.41              |
| 48:Z:33:ARG:NH2  | 48:Z:34:ARG:HD2   | 2.22                     | 0.41              |
| 49:a:3:LYS:HZ1   | 51:1:2106:U:H6    | 1.68                     | 0.41              |
| 50:3:392:C:H2'   | 50:3:393:A:H8     | 1.85                     | 0.41              |
| 50:3:1251:A:H2'  | 50:3:1252:A:C8    | 2.55                     | 0.41              |
| 51:1:741:U:H2'   | 51:1:742:A:C8     | 2.55                     | 0.41              |
| 51:1:1297:C:OP1  | 51:1:2710:C:H4'   | 2.20                     | 0.41              |
| 51:1:1328:A:H4'  | 51:1:1329:U:H5    | 1.85                     | 0.41              |
| 51:1:2306:C:H3'  | 51:1:2307:G:H5'   | 2.01                     | 0.41              |
| 10:m:64:TRP:O    | 10:m:104:GLU:N    | 2.53                     | 0.41              |
| 12:o:31:THR:HB   | 12:o:32:PRO:HD2   | 2.01                     | 0.41              |
| 30:H:142:ARG:HG3 | 30:H:143:LEU:HD22 | 2.02                     | 0.41              |
| 31:I:104:MET:HE2 | 31:I:170:LEU:HD22 | 2.01                     | 0.41              |
| 36:N:105:ARG:HG2 | 50:3:1117:A:O2'   | 2.20                     | 0.41              |
| 38:P:21:HIS:CE1  | 38:P:84:MET:HG2   | 2.55                     | 0.41              |
| 39:Q:31:GLY:HA3  | 39:Q:54:VAL:CG1   | 2.50                     | 0.41              |
| 39:Q:43:LYS:HB2  | 39:Q:44:PRO:HD3   | 2.01                     | 0.41              |
| 39:Q:52:CYS:O    | 39:Q:64:SER:N     | 2.49                     | 0.41              |
| 48:Z:14:ALA:HB1  | 48:Z:16:ARG:HG2   | 2.01                     | 0.41              |
| 50:3:114:U:O2'   | 50:3:115:G:H5'    | 2.21                     | 0.41              |
| 51:1:481:G:H1'   | 51:1:506:G:H21    | 1.84                     | 0.41              |
| 51:1:1137:G:H2'  | 51:1:1138:G:H8    | 1.85                     | 0.41              |
| 51:1:1378:A:H1'  | 51:1:1379:U:C5    | 2.55                     | 0.41              |
| 51:1:1764:C:O2'  | 51:1:1765:U:H5'   | 2.20                     | 0.41              |
| 51:1:1984:G:O2'  | 51:1:1985:C:H5'   | 2.21                     | 0.41              |
| 51:1:2022:U:O2'  | 51:1:2617:U:H5'   | 2.21                     | 0.41              |
| 1:b:166:ARG:HB3  | 1:b:166:ARG:NH1   | 2.35                     | 0.41              |
| 5:f:173:ALA:O    | 5:f:174:LYS:HB3   | 2.20                     | 0.41              |
| 7:j:55:ILE:HD13  | 7:j:132:HIS:CD2   | 2.55                     | 0.41              |
| 8:k:48:PRO:HA    | 50:3:1422:G:OP1   | 2.19                     | 0.41              |
| 12:o:107:ALA:O   | 12:o:111:ARG:HG3  | 2.21                     | 0.41              |
| 12:o:109:ALA:O   | 12:o:112:GLU:OE2  | 2.38                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:p:28:LYS:HD3  | 13:p:39:LEU:HD21 | 2.02                     | 0.41              |
| 14:q:32:ARG:HH11 | 51:1:1252:G:H4'  | 1.85                     | 0.41              |
| 16:s:23:LEU:HD11 | 24:B:21:LEU:HD22 | 2.03                     | 0.41              |
| 17:t:11:LEU:HD23 | 17:t:11:LEU:C    | 2.45                     | 0.41              |
| 31:I:33:ILE:O    | 31:I:34:GLU:HB2  | 2.20                     | 0.41              |
| 32:J:40:ASP:OD1  | 32:J:44:ARG:N    | 2.53                     | 0.41              |
| 35:M:21:LYS:HE2  | 50:3:827:U:H5''  | 2.02                     | 0.41              |
| 37:O:52:LEU:HD11 | 41:S:80:ARG:NE   | 2.34                     | 0.41              |
| 43:U:3:THR:HG23  | 43:U:66:THR:O    | 2.21                     | 0.41              |
| 47:Y:16:ALA:O    | 47:Y:20:ASN:ND2  | 2.53                     | 0.41              |
| 49:a:186:LYS:HA  | 49:a:189:LEU:HB2 | 2.01                     | 0.41              |
| 50:3:51:A:H4'    | 50:3:52:C:H5''   | 2.03                     | 0.41              |
| 50:3:707:U:H2'   | 50:3:708:C:C5    | 2.54                     | 0.41              |
| 51:1:43:G:H2'    | 51:1:44:A:O4'    | 2.20                     | 0.41              |
| 51:1:259:G:H2'   | 51:1:260:G:H8    | 1.84                     | 0.41              |
| 51:1:406:G:H2'   | 51:1:407:G:H8    | 1.84                     | 0.41              |
| 51:1:941:A:H2'   | 51:1:942:G:O4'   | 2.20                     | 0.41              |
| 51:1:1383:A:H2   | 51:1:1406:U:H1'  | 1.84                     | 0.41              |
| 51:1:1927:A:H2'  | 51:1:1928:A:O4'  | 2.19                     | 0.41              |
| 51:1:2019:A:H2   | 51:1:2035:G:H22  | 1.67                     | 0.41              |
| 51:1:2036:C:H2'  | 51:1:2037:A:C8   | 2.55                     | 0.41              |
| 51:1:2556:C:H2'  | 51:1:2557:G:O4'  | 2.21                     | 0.41              |
| 51:1:2690:U:O2'  | 51:1:2872:A:H1'  | 2.20                     | 0.41              |
| 52:2:101:A:H2'   | 52:2:102:G:O4'   | 2.20                     | 0.41              |
| 54:4:17:U:O2'    | 54:4:18:G:H5'    | 2.20                     | 0.41              |
| 55:8:12:GLN:O    | 55:8:16:GLU:HG2  | 2.20                     | 0.41              |
| 1:b:128:THR:HG22 | 1:b:188:ARG:HB3  | 2.02                     | 0.41              |
| 2:c:38:LYS:HB3   | 2:c:43:ASP:OD2   | 2.19                     | 0.41              |
| 4:e:106:ALA:N    | 4:e:108:PRO:HD2  | 2.36                     | 0.41              |
| 4:e:153:ILE:HG23 | 4:e:153:ILE:O    | 2.20                     | 0.41              |
| 9:l:54:GLN:HE22  | 51:1:2358:A:N6   | 2.10                     | 0.41              |
| 11:n:78:LYS:O    | 11:n:82:GLU:HB2  | 2.20                     | 0.41              |
| 13:p:29:VAL:HB   | 13:p:40:GLN:HB3  | 2.02                     | 0.41              |
| 14:q:38:VAL:HG13 | 14:q:39:ILE:N    | 2.35                     | 0.41              |
| 16:s:90:LYS:HA   | 51:1:751:A:H5'   | 2.03                     | 0.41              |
| 18:u:81:ARG:HG3  | 18:u:96:LYS:HG3  | 2.02                     | 0.41              |
| 21:x:36:ARG:HA   | 21:x:47:THR:HA   | 2.02                     | 0.41              |
| 22:y:41:HIS:CE1  | 22:y:42:LEU:HG   | 2.55                     | 0.41              |
| 31:I:159:GLU:HA  | 31:I:162:GLU:OE1 | 2.20                     | 0.41              |
| 40:R:32:ILE:HG23 | 40:R:58:GLU:CG   | 2.50                     | 0.41              |
| 50:3:211:G:H3'   | 50:3:211:G:N3    | 2.35                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:3:416:G:O2'    | 50:3:417:G:H5'    | 2.21                     | 0.41              |
| 50:3:1306:A:H2'   | 50:3:1307:U:O4'   | 2.19                     | 0.41              |
| 51:1:457:A:N1     | 51:1:470:A:H5''   | 2.35                     | 0.41              |
| 51:1:1086:A:H4'   | 51:1:1103:A:N1    | 2.35                     | 0.41              |
| 51:1:1685:C:H2'   | 51:1:1686:C:C6    | 2.55                     | 0.41              |
| 51:1:2368:C:H2'   | 51:1:2369:A:H8    | 1.86                     | 0.41              |
| 2:c:116:LYS:HG3   | 2:c:165:MET:HE2   | 2.02                     | 0.41              |
| 7:j:105:VAL:HG21  | 7:j:122:LEU:CD2   | 2.50                     | 0.41              |
| 7:j:111:LYS:HE3   | 7:j:111:LYS:HB2   | 1.93                     | 0.41              |
| 12:o:92:PHE:HB2   | 12:o:117:PHE:CD2  | 2.56                     | 0.41              |
| 14:q:24:TYR:HB3   | 51:1:533:G:OP1    | 2.20                     | 0.41              |
| 24:B:5:ASN:O      | 24:B:7:PRO:HD3    | 2.19                     | 0.41              |
| 30:H:85:LYS:NZ    | 30:H:89:VAL:HG11  | 2.35                     | 0.41              |
| 31:I:2:ARG:HD3    | 31:I:2:ARG:N      | 2.35                     | 0.41              |
| 31:I:90:LEU:CD1   | 31:I:190:LEU:HD22 | 2.50                     | 0.41              |
| 31:I:124:VAL:O    | 31:I:124:VAL:HG13 | 2.20                     | 0.41              |
| 31:I:158:LEU:HD12 | 31:I:159:GLU:N    | 2.35                     | 0.41              |
| 32:J:60:GLN:O     | 32:J:64:GLU:HG3   | 2.21                     | 0.41              |
| 32:J:156:ARG:O    | 32:J:158:LYS:N    | 2.45                     | 0.41              |
| 34:L:20:GLU:O     | 34:L:24:LYS:N     | 2.49                     | 0.41              |
| 36:N:5:TYR:HB2    | 36:N:20:ILE:CG2   | 2.50                     | 0.41              |
| 48:Z:6:ARG:O      | 48:Z:7:GLU:C      | 2.63                     | 0.41              |
| 50:3:273:U:O2'    | 50:3:274:A:H5'    | 2.20                     | 0.41              |
| 50:3:411:A:H1'    | 50:3:413:G:N9     | 2.35                     | 0.41              |
| 50:3:600:A:H2'    | 50:3:601:G:C8     | 2.54                     | 0.41              |
| 50:3:1128:C:H1'   | 50:3:1148:U:H3    | 1.85                     | 0.41              |
| 50:3:1354:U:H2'   | 50:3:1355:G:C8    | 2.55                     | 0.41              |
| 50:3:1407:C:O2'   | 50:3:1408:A:H5'   | 2.21                     | 0.41              |
| 50:3:1494:G:O2'   | 50:3:1495:U:H5'   | 2.20                     | 0.41              |
| 51:1:49:A:H2'     | 51:1:49:A:N3      | 2.34                     | 0.41              |
| 51:1:720:U:H2'    | 51:1:721:A:C8     | 2.54                     | 0.41              |
| 51:1:905:A:H2'    | 51:1:906:U:H5'    | 2.02                     | 0.41              |
| 51:1:912:C:O2'    | 51:1:913:U:H5'    | 2.20                     | 0.41              |
| 51:1:1595:C:H2'   | 51:1:1596:A:C8    | 2.56                     | 0.41              |
| 51:1:1854:A:H2'   | 51:1:1855:U:H5'   | 2.02                     | 0.41              |
| 51:1:2283:C:H2'   | 51:1:2284:A:O4'   | 2.20                     | 0.41              |
| 51:1:2304:G:C2'   | 51:1:2305:U:H5'   | 2.50                     | 0.41              |
| 51:1:2345:G:H21   | 51:1:2381:A:H3'   | 1.85                     | 0.41              |
| 51:1:2359:C:O2'   | 51:1:2360:G:H5'   | 2.19                     | 0.41              |
| 51:1:2498:C:H6    | 51:1:2498:C:H5'   | 1.84                     | 0.41              |
| 52:2:97:C:H2'     | 52:2:98:G:O4'     | 2.20                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:b:262:THR:OG1  | 1:b:265:PHE:HD2   | 2.03                     | 0.41              |
| 2:c:24:VAL:HG23  | 2:c:189:VAL:O     | 2.21                     | 0.41              |
| 3:d:154:ASP:OD2  | 3:d:157:LEU:HD13  | 2.21                     | 0.41              |
| 3:d:155:GLU:HG3  | 3:d:159:LEU:HG    | 2.02                     | 0.41              |
| 4:e:65:LEU:N     | 4:e:87:LYS:O      | 2.54                     | 0.41              |
| 5:f:64:ALA:O     | 5:f:68:ARG:N      | 2.52                     | 0.41              |
| 5:f:138:GLN:HA   | 51:1:2745:C:O2'   | 2.21                     | 0.41              |
| 7:j:7:LYS:HA     | 7:j:8:PRO:HD3     | 1.94                     | 0.41              |
| 10:m:108:VAL:HB  | 10:m:109:PRO:HD2  | 2.02                     | 0.41              |
| 11:n:94:TYR:O    | 11:n:116:VAL:HG22 | 2.21                     | 0.41              |
| 15:r:35:PHE:HB2  | 15:r:59:ILE:HB    | 2.02                     | 0.41              |
| 18:u:6:ARG:HG3   | 18:u:7:ASP:H      | 1.86                     | 0.41              |
| 19:v:61:LEU:N    | 19:v:72:VAL:O     | 2.53                     | 0.41              |
| 23:z:19:HIS:ND1  | 23:z:50:VAL:HG12  | 2.36                     | 0.41              |
| 29:G:45:THR:HB   | 29:G:200:PRO:HD2  | 2.02                     | 0.41              |
| 37:O:40:ILE:HG22 | 37:O:42:LEU:HG    | 2.03                     | 0.41              |
| 38:P:34:THR:HA   | 38:P:40:ALA:HA    | 2.02                     | 0.41              |
| 40:R:10:ASP:O    | 40:R:12:LYS:HG2   | 2.20                     | 0.41              |
| 40:R:89:ARG:HG3  | 40:R:89:ARG:HH11  | 1.86                     | 0.41              |
| 42:T:46:LYS:O    | 42:T:52:ARG:NH2   | 2.54                     | 0.41              |
| 43:U:21:VAL:HG13 | 43:U:33:ILE:HB    | 2.02                     | 0.41              |
| 47:Y:59:ARG:NH1  | 50:3:177:G:H5'    | 2.36                     | 0.41              |
| 50:3:959:A:H2'   | 50:3:960:U:C4'    | 2.46                     | 0.41              |
| 50:3:1188:A:H2'  | 50:3:1189:U:H5'   | 2.03                     | 0.41              |
| 51:1:44:A:H2'    | 51:1:45:G:O4'     | 2.21                     | 0.41              |
| 51:1:639:U:H2'   | 51:1:640:C:C6     | 2.55                     | 0.41              |
| 55:8:125:SER:HA  | 55:8:187:TYR:N    | 2.33                     | 0.41              |
| 1:b:203:VAL:HG13 | 1:b:203:VAL:O     | 2.21                     | 0.41              |
| 3:d:161:ALA:HB3  | 3:d:169:VAL:HG23  | 2.01                     | 0.41              |
| 4:e:103:ILE:HD12 | 4:e:172:PHE:CG    | 2.56                     | 0.41              |
| 4:e:109:ARG:NH1  | 4:e:110:ILE:HA    | 2.35                     | 0.41              |
| 5:f:11:PRO:HB2   | 5:f:14:VAL:HG21   | 2.02                     | 0.41              |
| 6:g:11:ASN:HD22  | 51:1:2095:A:C5'   | 2.34                     | 0.41              |
| 10:m:3:GLN:HA    | 10:m:4:PRO:HD3    | 1.77                     | 0.41              |
| 11:n:22:ARG:HH12 | 51:1:2709:G:C5'   | 2.32                     | 0.41              |
| 11:n:74:GLU:O    | 11:n:77:ALA:HB3   | 2.21                     | 0.41              |
| 15:r:79:ARG:HD2  | 15:r:80:ARG:NH1   | 2.35                     | 0.41              |
| 20:w:16:ARG:HH11 | 20:w:16:ARG:HG3   | 1.85                     | 0.41              |
| 25:C:35:LEU:HD23 | 25:C:37:LYS:HD2   | 2.03                     | 0.41              |
| 29:G:54:ALA:O    | 29:G:57:ASN:HB2   | 2.21                     | 0.41              |
| 30:H:85:LYS:HD3  | 30:H:85:LYS:C     | 2.46                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:I:10:LEU:H    | 31:I:10:LEU:CD2   | 2.30                     | 0.41              |
| 32:J:95:MET:HA   | 32:J:124:ALA:HA   | 2.03                     | 0.41              |
| 32:J:149:PRO:C   | 32:J:152:VAL:HG22 | 2.46                     | 0.41              |
| 36:N:4:GLN:HA    | 36:N:21:LYS:HG2   | 2.02                     | 0.41              |
| 40:R:27:THR:HB   | 50:3:1328:C:OP1   | 2.21                     | 0.41              |
| 41:S:100:TRP:O   | 50:3:1186:G:N2    | 2.49                     | 0.41              |
| 48:Z:53:LYS:HA   | 48:Z:56:ALA:HB3   | 2.02                     | 0.41              |
| 50:3:604:G:H2'   | 50:3:605:U:O4'    | 2.20                     | 0.41              |
| 50:3:696:A:O2'   | 50:3:697:U:H5'    | 2.21                     | 0.41              |
| 50:3:872:A:H2'   | 50:3:872:A:N3     | 2.36                     | 0.41              |
| 50:3:936:C:O2'   | 50:3:937:A:H5'    | 2.21                     | 0.41              |
| 51:1:214:G:O2'   | 51:1:215:G:H5'    | 2.20                     | 0.41              |
| 51:1:582:A:H2'   | 51:1:583:G:H8     | 1.85                     | 0.41              |
| 51:1:1021:A:H3'  | 51:1:1021:A:N3    | 2.34                     | 0.41              |
| 51:1:1147:A:O2'  | 51:1:1148:U:H5'   | 2.20                     | 0.41              |
| 51:1:1564:C:H2'  | 51:1:1565:C:O4'   | 2.20                     | 0.41              |
| 51:1:2368:C:H2'  | 51:1:2369:A:C8    | 2.55                     | 0.41              |
| 51:1:2443:C:H2'  | 51:1:2444:G:C8    | 2.55                     | 0.41              |
| 51:1:2849:U:H4'  | 51:1:2868:A:N1    | 2.36                     | 0.41              |
| 54:4:21:A:H62    | 55:8:215:THR:CG2  | 2.34                     | 0.41              |
| 3:d:95:LYS:HG2   | 3:d:96:VAL:N      | 2.36                     | 0.41              |
| 4:e:75:GLY:HA3   | 51:1:2311:A:N3    | 2.36                     | 0.41              |
| 5:f:1:SER:N      | 51:1:2749:A:OP1   | 2.54                     | 0.41              |
| 5:f:8:VAL:O      | 5:f:48:THR:HG23   | 2.21                     | 0.41              |
| 5:f:125:PRO:HG2  | 5:f:126:THR:N     | 2.35                     | 0.41              |
| 17:t:50:LEU:HD21 | 22:y:26:PHE:CG    | 2.56                     | 0.41              |
| 19:v:40:ILE:HG22 | 19:v:42:LEU:CD2   | 2.50                     | 0.41              |
| 19:v:47:VAL:HG23 | 19:v:86:LEU:HD12  | 2.03                     | 0.41              |
| 20:w:7:ARG:HH22  | 53:5:2:G:H5'      | 1.86                     | 0.41              |
| 21:x:48:LEU:HD21 | 21:x:77:TYR:HB2   | 2.02                     | 0.41              |
| 27:E:61:LEU:O    | 27:E:61:LEU:HG    | 2.20                     | 0.41              |
| 29:G:11:ALA:HB2  | 29:G:211:LEU:HG   | 2.02                     | 0.41              |
| 29:G:12:GLY:HA2  | 29:G:14:HIS:CE1   | 2.56                     | 0.41              |
| 29:G:186:VAL:CG1 | 29:G:190:SER:HB2  | 2.48                     | 0.41              |
| 30:H:28:PHE:O    | 30:H:32:LEU:HD13  | 2.21                     | 0.41              |
| 31:I:36:ALA:H    | 31:I:37:PRO:HD3   | 1.84                     | 0.41              |
| 31:I:51:GLY:O    | 31:I:54:LEU:HB3   | 2.21                     | 0.41              |
| 32:J:18:ASN:ND2  | 50:3:17:U:OP1     | 2.54                     | 0.41              |
| 33:K:53:LYS:HE2  | 33:K:53:LYS:HB2   | 1.92                     | 0.41              |
| 36:N:30:ASN:OD1  | 36:N:66:VAL:HG12  | 2.21                     | 0.41              |
| 37:O:37:ARG:HH21 | 50:3:1124:G:H3'   | 1.85                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 38:P:43:TRP:HE3   | 50:3:705:G:H22   | 1.67                     | 0.41              |
| 40:R:33:LEU:CD1   | 40:R:38:ILE:HB   | 2.48                     | 0.41              |
| 40:R:70:ARG:O     | 40:R:74:MET:HB2  | 2.21                     | 0.41              |
| 42:T:80:LEU:HA    | 42:T:83:ARG:HB3  | 2.03                     | 0.41              |
| 47:Y:2:ASN:ND2    | 47:Y:3:ILE:H     | 2.19                     | 0.41              |
| 50:3:162:A:C2'    | 50:3:163:C:H5'   | 2.51                     | 0.41              |
| 50:3:320:A:H2'    | 50:3:321:A:C8    | 2.56                     | 0.41              |
| 50:3:484:G:H4'    | 50:3:485:U:C5'   | 2.41                     | 0.41              |
| 51:1:186:G:H2'    | 51:1:187:G:C8    | 2.56                     | 0.41              |
| 51:1:389:G:C2'    | 51:1:390:U:H5'   | 2.50                     | 0.41              |
| 51:1:807:U:H2'    | 51:1:808:G:C8    | 2.55                     | 0.41              |
| 51:1:854:C:O2'    | 51:1:855:G:H5'   | 2.20                     | 0.41              |
| 51:1:970:U:H2'    | 51:1:971:G:C8    | 2.55                     | 0.41              |
| 51:1:1367:A:H2'   | 51:1:1368:G:C5'  | 2.43                     | 0.41              |
| 51:1:1558:C:C5'   | 51:1:1559:U:H3'  | 2.49                     | 0.41              |
| 51:1:1563:U:H2'   | 51:1:1564:C:C6   | 2.56                     | 0.41              |
| 51:1:2287:A:O2'   | 51:1:2288:A:H2'  | 2.20                     | 0.41              |
| 51:1:2748:A:H2'   | 51:1:2749:A:O4'  | 2.21                     | 0.41              |
| 55:8:173:VAL:HG23 | 55:8:174:ALA:H   | 1.86                     | 0.41              |
| 1:b:140:VAL:HG12  | 1:b:191:LEU:HA   | 2.03                     | 0.41              |
| 1:b:200:MET:HE3   | 51:1:1820:U:C2   | 2.56                     | 0.41              |
| 1:b:216:ARG:NH2   | 51:1:781:A:OP1   | 2.54                     | 0.41              |
| 2:c:25:THR:HG21   | 2:c:193:VAL:HG22 | 2.01                     | 0.41              |
| 3:d:21:ARG:NH2    | 3:d:106:LYS:HB2  | 2.36                     | 0.41              |
| 3:d:147:LEU:HD13  | 3:d:183:PHE:CD2  | 2.56                     | 0.41              |
| 3:d:149:ILE:CG2   | 3:d:188:MET:HA   | 2.47                     | 0.41              |
| 3:d:176:ASP:OD2   | 3:d:178:VAL:CG2  | 2.69                     | 0.41              |
| 6:g:4:ILE:HD11    | 6:g:43:ASN:HB3   | 2.02                     | 0.41              |
| 7:j:27:ARG:O      | 7:j:31:GLU:HG2   | 2.20                     | 0.41              |
| 9:l:57:LEU:HA     | 9:l:60:ARG:HH11  | 1.86                     | 0.41              |
| 10:m:135:VAL:HG12 | 19:v:79:ARG:NH2  | 2.30                     | 0.41              |
| 14:q:24:TYR:HE1   | 51:1:17:G:H4'    | 1.86                     | 0.41              |
| 29:G:187:ASP:H    | 29:G:190:SER:HB2 | 1.86                     | 0.41              |
| 31:I:151:GLN:O    | 31:I:152:SER:OG  | 2.34                     | 0.41              |
| 33:K:86:ARG:NH2   | 50:3:673:A:O2'   | 2.54                     | 0.41              |
| 34:L:37:THR:HG22  | 50:3:1291:U:P    | 2.61                     | 0.41              |
| 35:M:7:ALA:O      | 35:M:11:THR:N    | 2.54                     | 0.41              |
| 35:M:47:ASP:N     | 35:M:61:THR:HB   | 2.35                     | 0.41              |
| 36:N:51:LEU:HD13  | 36:N:56:MET:CG   | 2.39                     | 0.41              |
| 36:N:91:GLU:OE1   | 36:N:94:ARG:CB   | 2.69                     | 0.41              |
| 36:N:118:ARG:HH12 | 50:3:1233:G:H5'  | 1.86                     | 0.41              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 38:P:63:GLN:HG3  | 38:P:98:ALA:HB2 | 2.02                     | 0.41              |
| 38:P:124:LYS:NZ  | 48:Z:33:ARG:O   | 2.54                     | 0.41              |
| 46:X:5:LYS:HE2   | 50:3:1313:U:OP1 | 2.20                     | 0.41              |
| 47:Y:28:ARG:O    | 47:Y:32:LYS:HG2 | 2.21                     | 0.41              |
| 48:Z:19:LYS:O    | 48:Z:24:LYS:HG2 | 2.20                     | 0.41              |
| 50:3:31:G:H5'    | 50:3:306:A:C2   | 2.55                     | 0.41              |
| 50:3:162:A:H2'   | 50:3:163:C:O4'  | 2.20                     | 0.41              |
| 50:3:396:C:H2'   | 50:3:397:A:H5'' | 2.02                     | 0.41              |
| 50:3:493:A:H2'   | 50:3:494:G:C8   | 2.56                     | 0.41              |
| 50:3:505:G:H2'   | 50:3:506:G:H8   | 1.86                     | 0.41              |
| 50:3:613:C:H2'   | 50:3:614:C:C6   | 2.56                     | 0.41              |
| 50:3:751:U:H2'   | 50:3:752:G:O4'  | 2.21                     | 0.41              |
| 50:3:975:A:H1'   | 50:3:1358:U:H4' | 2.01                     | 0.41              |
| 50:3:1097:C:H2'  | 50:3:1098:C:C6  | 2.56                     | 0.41              |
| 51:1:68:G:H2'    | 51:1:69:C:O4'   | 2.21                     | 0.41              |
| 51:1:325:G:H2'   | 51:1:326:G:C8   | 2.56                     | 0.41              |
| 51:1:445:C:C2'   | 51:1:446:G:H5'  | 2.51                     | 0.41              |
| 51:1:680:C:H2'   | 51:1:681:G:H8   | 1.86                     | 0.41              |
| 51:1:1655:A:C2   | 51:1:2049:G:H4' | 2.56                     | 0.41              |
| 51:1:1683:U:H2'  | 51:1:1684:G:H8  | 1.86                     | 0.41              |
| 51:1:1745:A:H2'  | 51:1:1746:A:C8  | 2.56                     | 0.41              |
| 51:1:1912:A:N6   | 51:1:1917:U:H3  | 2.07                     | 0.41              |
| 51:1:2364:C:H2'  | 51:1:2365:G:O4' | 2.21                     | 0.41              |
| 51:1:2380:C:H2'  | 51:1:2381:A:H8  | 1.86                     | 0.41              |
| 51:1:2583:G:C2'  | 51:1:2584:U:H5' | 2.50                     | 0.41              |
| 52:2:12:C:H1'    | 52:2:15:A:C6    | 2.56                     | 0.41              |
| 54:4:17:U:H2'    | 54:4:18:G:C8    | 2.55                     | 0.41              |
| 1:b:143:VAL:HG22 | 1:b:189:ALA:HB1 | 2.02                     | 0.41              |
| 2:c:45:TYR:HB2   | 2:c:83:ARG:NH1  | 2.36                     | 0.41              |
| 3:d:48:THR:C     | 3:d:50:ALA:H    | 2.29                     | 0.41              |
| 4:e:109:ARG:CD   | 4:e:136:ILE:HA  | 2.47                     | 0.41              |
| 6:g:135:HIS:CD2  | 6:g:136:SER:H   | 2.38                     | 0.41              |
| 7:j:9:GLU:H      | 7:j:9:GLU:CD    | 2.28                     | 0.41              |
| 7:j:65:THR:HG22  | 51:1:1141:U:OP2 | 2.20                     | 0.41              |
| 9:l:50:PHE:CZ    | 9:l:52:GLY:HA2  | 2.56                     | 0.41              |
| 14:q:21:LYS:HG2  | 51:1:19:A:H5''  | 2.02                     | 0.41              |
| 14:q:109:VAL:O   | 14:q:113:LYS:N  | 2.48                     | 0.41              |
| 17:t:54:GLU:HB2  | 17:t:88:LYS:HD2 | 2.02                     | 0.41              |
| 25:C:9:LYS:HG3   | 25:C:19:PHE:CD2 | 2.56                     | 0.41              |
| 25:C:25:ASN:ND2  | 25:C:28:THR:OG1 | 2.54                     | 0.41              |
| 26:D:31:LEU:O    | 26:D:35:ARG:HG3 | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:I:56:GLU:OE1  | 31:I:194:ILE:HB   | 2.20                     | 0.41              |
| 33:K:6:ILE:HG12  | 33:K:89:VAL:HG22  | 2.02                     | 0.41              |
| 34:L:110:ARG:HG2 | 34:L:110:ARG:NH1  | 2.35                     | 0.41              |
| 36:N:86:LEU:HD13 | 36:N:97:LEU:HD11  | 2.03                     | 0.41              |
| 39:Q:34:THR:O    | 39:Q:53:ARG:HB3   | 2.20                     | 0.41              |
| 39:Q:120:ARG:HB2 | 50:3:37:U:OP1     | 2.20                     | 0.41              |
| 47:Y:14:GLU:O    | 47:Y:17:ARG:HG2   | 2.21                     | 0.41              |
| 47:Y:54:GLN:NE2  | 50:3:193:C:H1'    | 2.36                     | 0.41              |
| 48:Z:11:PHE:O    | 48:Z:13:VAL:N     | 2.54                     | 0.41              |
| 49:a:188:ASN:O   | 49:a:192:LEU:N    | 2.54                     | 0.41              |
| 50:3:243:A:H4'   | 50:3:244:U:H3'    | 2.03                     | 0.41              |
| 50:3:600:A:H2'   | 50:3:601:G:H8     | 1.86                     | 0.41              |
| 50:3:823:C:H2'   | 50:3:824:G:H8     | 1.86                     | 0.41              |
| 50:3:1175:G:H2'  | 50:3:1176:A:C8    | 2.56                     | 0.41              |
| 50:3:1293:C:H2'  | 50:3:1294:G:H8    | 1.85                     | 0.41              |
| 51:1:807:U:O2'   | 51:1:808:G:H5'    | 2.21                     | 0.41              |
| 51:1:1511:G:H2'  | 51:1:1512:C:C6    | 2.55                     | 0.41              |
| 51:1:2070:A:O2'  | 51:1:2071:A:H5'   | 2.21                     | 0.41              |
| 52:2:2:G:H2'     | 52:2:3:C:C6       | 2.56                     | 0.41              |
| 2:c:128:ARG:NH1  | 51:1:1996:C:H5''  | 2.37                     | 0.40              |
| 10:m:18:ARG:HG3  | 10:m:18:ARG:HH21  | 1.87                     | 0.40              |
| 10:m:60:GLN:H    | 10:m:60:GLN:HG2   | 1.59                     | 0.40              |
| 11:n:47:VAL:O    | 11:n:50:PRO:HD2   | 2.20                     | 0.40              |
| 16:s:29:VAL:CG1  | 16:s:55:ILE:HD11  | 2.50                     | 0.40              |
| 21:x:46:VAL:HG23 | 21:x:46:VAL:O     | 2.21                     | 0.40              |
| 24:B:13:GLY:HA3  | 51:1:16:C:C5'     | 2.48                     | 0.40              |
| 29:G:68:PHE:O    | 29:G:91:VAL:HG12  | 2.21                     | 0.40              |
| 31:I:18:LEU:HB2  | 31:I:20:LEU:HG    | 2.02                     | 0.40              |
| 32:J:148:SER:HB2 | 32:J:149:PRO:HD2  | 2.03                     | 0.40              |
| 35:M:76:ARG:HH11 | 35:M:76:ARG:HG2   | 1.85                     | 0.40              |
| 36:N:105:ARG:HG3 | 36:N:105:ARG:NH1  | 2.36                     | 0.40              |
| 37:O:17:LEU:HD21 | 37:O:93:ALA:HB1   | 2.03                     | 0.40              |
| 40:R:16:ILE:HA   | 40:R:26:LYS:HZ3   | 1.86                     | 0.40              |
| 40:R:22:TYR:CD1  | 50:3:1330:U:H4'   | 2.56                     | 0.40              |
| 42:T:31:LEU:HD12 | 42:T:31:LEU:N     | 2.36                     | 0.40              |
| 46:X:10:ILE:HG23 | 46:X:40:PHE:CE2   | 2.56                     | 0.40              |
| 49:a:27:ILE:HG13 | 49:a:185:LEU:HD22 | 2.03                     | 0.40              |
| 50:3:398:U:H2'   | 50:3:399:G:H8     | 1.86                     | 0.40              |
| 50:3:1131:G:N2   | 50:3:1144:G:H4'   | 2.36                     | 0.40              |
| 51:1:114:U:H5'   | 51:1:114:U:C6     | 2.53                     | 0.40              |
| 51:1:393:C:H2'   | 51:1:394:C:C6     | 2.56                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 51:1:672:C:O2'   | 51:1:673:C:H5'    | 2.20                     | 0.40              |
| 51:1:1690:A:H2'  | 51:1:1691:C:O4'   | 2.21                     | 0.40              |
| 51:1:2262:U:H2'  | 51:1:2263:C:H6    | 1.86                     | 0.40              |
| 51:1:2267:A:H61  | 51:1:2272:U:H3    | 1.69                     | 0.40              |
| 51:1:2306:C:H3'  | 51:1:2307:G:C5'   | 2.51                     | 0.40              |
| 51:1:2853:C:H2'  | 51:1:2854:G:C8    | 2.56                     | 0.40              |
| 4:e:39:VAL:HG12  | 4:e:41:GLU:HG2    | 2.03                     | 0.40              |
| 5:f:136:ASP:O    | 5:f:140:ILE:HG12  | 2.21                     | 0.40              |
| 6:g:128:HIS:CG   | 6:g:129:GLU:H     | 2.40                     | 0.40              |
| 7:j:105:VAL:HG21 | 7:j:122:LEU:HD22  | 2.02                     | 0.40              |
| 8:k:4:GLU:H      | 8:k:4:GLU:CD      | 2.28                     | 0.40              |
| 10:m:67:VAL:HG12 | 10:m:100:LYS:HE3  | 2.02                     | 0.40              |
| 11:n:59:SER:O    | 11:n:63:ARG:HG3   | 2.21                     | 0.40              |
| 29:G:187:ASP:H   | 29:G:190:SER:CB   | 2.34                     | 0.40              |
| 30:H:6:PRO:HG3   | 30:H:174:LEU:HD11 | 2.04                     | 0.40              |
| 30:H:13:ILE:HD11 | 50:3:1113:C:O2'   | 2.22                     | 0.40              |
| 31:I:137:SER:O   | 31:I:140:ASP:OD2  | 2.39                     | 0.40              |
| 32:J:28:ARG:HG3  | 32:J:28:ARG:HH11  | 1.87                     | 0.40              |
| 32:J:108:GLY:O   | 32:J:109:ALA:CB   | 2.68                     | 0.40              |
| 33:K:75:GLU:HA   | 33:K:78:PHE:HD2   | 1.85                     | 0.40              |
| 34:L:22:LEU:HD21 | 34:L:46:LEU:HD21  | 2.02                     | 0.40              |
| 34:L:65:LEU:HA   | 34:L:68:VAL:HG22  | 2.03                     | 0.40              |
| 38:P:79:LYS:O    | 38:P:105:ARG:N    | 2.50                     | 0.40              |
| 39:Q:38:THR:CG2  | 39:Q:48:LEU:HB3   | 2.50                     | 0.40              |
| 39:Q:55:ARG:HG2  | 39:Q:55:ARG:HH21  | 1.87                     | 0.40              |
| 39:Q:97:VAL:CG2  | 39:Q:100:ALA:HB2  | 2.32                     | 0.40              |
| 39:Q:115:LYS:O   | 39:Q:116:TYR:CB   | 2.70                     | 0.40              |
| 43:U:14:ARG:HH11 | 43:U:14:ARG:HG3   | 1.86                     | 0.40              |
| 45:W:36:GLY:O    | 45:W:62:ARG:NH2   | 2.55                     | 0.40              |
| 50:3:505:G:H2'   | 50:3:506:G:C8     | 2.56                     | 0.40              |
| 50:3:960:U:O2'   | 50:3:1223:C:H5'   | 2.22                     | 0.40              |
| 50:3:993:G:H21   | 50:3:996:A:N6     | 2.00                     | 0.40              |
| 50:3:997:U:H2'   | 50:3:998:C:C6     | 2.55                     | 0.40              |
| 50:3:1420:U:H2'  | 50:3:1421:G:H8    | 1.86                     | 0.40              |
| 51:1:548:G:C5    | 51:1:549:G:H1'    | 2.56                     | 0.40              |
| 51:1:1558:C:H5'' | 51:1:1559:U:H6    | 1.86                     | 0.40              |
| 51:1:1584:U:C5   | 51:1:1585:C:H1'   | 2.56                     | 0.40              |
| 51:1:1826:G:H2'  | 51:1:1827:U:C6    | 2.56                     | 0.40              |
| 51:1:1998:A:H2'  | 51:1:1999:C:C6    | 2.57                     | 0.40              |
| 51:1:2455:G:H2'  | 51:1:2456:C:C6    | 2.55                     | 0.40              |
| 55:8:123:TYR:HB3 | 55:8:126:ALA:HB3  | 2.02                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:8:243:VAL:HG11 | 55:8:280:GLN:HE21 | 1.86                     | 0.40              |
| 1:b:52:HIS:ND1    | 1:b:218:THR:HG22  | 2.36                     | 0.40              |
| 1:b:262:THR:HG21  | 51:1:1800:C:OP2   | 2.22                     | 0.40              |
| 2:c:148:GLN:HB3   | 51:1:2574:G:O2'   | 2.21                     | 0.40              |
| 2:c:179:ARG:HH11  | 2:c:179:ARG:CB    | 2.35                     | 0.40              |
| 2:c:180:VAL:HG23  | 2:c:180:VAL:O     | 2.21                     | 0.40              |
| 4:e:87:LYS:HZ1    | 51:1:2313:C:C3'   | 2.35                     | 0.40              |
| 5:f:161:VAL:HG22  | 5:f:162:ARG:N     | 2.36                     | 0.40              |
| 8:k:24:VAL:HG13   | 8:k:24:VAL:O      | 2.21                     | 0.40              |
| 10:m:41:LEU:HD23  | 10:m:96:ILE:CG1   | 2.50                     | 0.40              |
| 14:q:87:VAL:HG12  | 14:q:89:ILE:H     | 1.86                     | 0.40              |
| 15:r:79:ARG:O     | 15:r:81:LYS:N     | 2.55                     | 0.40              |
| 21:x:17:ARG:HG2   | 51:1:380:G:H5'    | 2.03                     | 0.40              |
| 30:H:25:THR:HA    | 41:S:75:LYS:HE3   | 2.02                     | 0.40              |
| 32:J:86:GLY:N     | 32:J:93:VAL:O     | 2.36                     | 0.40              |
| 32:J:159:SER:OG   | 32:J:162:GLU:HB3  | 2.22                     | 0.40              |
| 33:K:11:HIS:HB3   | 33:K:83:ALA:HB1   | 2.02                     | 0.40              |
| 34:L:58:LEU:H     | 34:L:58:LEU:CD1   | 2.27                     | 0.40              |
| 35:M:91:LEU:HD12  | 35:M:116:ARG:HG2  | 2.03                     | 0.40              |
| 36:N:56:MET:SD    | 36:N:56:MET:C     | 3.05                     | 0.40              |
| 39:Q:65:TYR:HB2   | 39:Q:92:VAL:HG11  | 2.02                     | 0.40              |
| 39:Q:110:LYS:CG   | 50:3:538:G:H5''   | 2.51                     | 0.40              |
| 41:S:85:GLU:HA    | 41:S:88:MET:HB2   | 2.04                     | 0.40              |
| 48:Z:40:PRO:HA    | 48:Z:43:GLU:HB3   | 2.04                     | 0.40              |
| 50:3:160:A:H1'    | 50:3:344:A:C6     | 2.56                     | 0.40              |
| 50:3:220:G:O2'    | 50:3:221:C:H5'    | 2.21                     | 0.40              |
| 50:3:1218:C:H2'   | 50:3:1219:A:H8    | 1.86                     | 0.40              |
| 50:3:1391:U:H2'   | 50:3:1392:G:H8    | 1.86                     | 0.40              |
| 51:1:103:A:H2'    | 51:1:104:A:O4'    | 2.20                     | 0.40              |
| 51:1:306:U:H2'    | 51:1:307:G:O4'    | 2.22                     | 0.40              |
| 51:1:1161:C:H2'   | 51:1:1162:G:H8    | 1.87                     | 0.40              |
| 51:1:1282:U:H2'   | 51:1:1283:G:O4'   | 2.22                     | 0.40              |
| 51:1:1870:C:C3'   | 51:1:1871:A:H5'   | 2.52                     | 0.40              |
| 51:1:2832:U:H1'   | 51:1:2834:G:C2    | 2.57                     | 0.40              |
| 55:8:128:CYS:HB3  | 55:8:189:TYR:CB   | 2.50                     | 0.40              |
| 2:c:105:LYS:O     | 2:c:177:VAL:HG12  | 2.21                     | 0.40              |
| 4:e:33:ILE:HG13   | 4:e:95:MET:HG3    | 2.03                     | 0.40              |
| 6:g:97:ARG:HE     | 6:g:100:ALA:HB3   | 1.87                     | 0.40              |
| 7:j:25:LEU:HD13   | 7:j:62:VAL:HG11   | 2.03                     | 0.40              |
| 10:m:51:ARG:HH12  | 51:1:2483:C:H4'   | 1.87                     | 0.40              |
| 10:m:58:LYS:O     | 10:m:59:ARG:HB2   | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:q:111:LYS:HE3  | 15:r:49:ILE:O     | 2.22                     | 0.40              |
| 18:u:47:PRO:HG3   | 51:1:484:C:OP1    | 2.21                     | 0.40              |
| 29:G:160:LEU:HG   | 29:G:180:ILE:HD11 | 2.03                     | 0.40              |
| 29:G:210:THR:HA   | 29:G:213:LEU:HG   | 2.04                     | 0.40              |
| 30:H:155:ARG:HG3  | 30:H:155:ARG:NH1  | 2.36                     | 0.40              |
| 33:K:91:ARG:HH21  | 45:W:56:ARG:NE    | 2.17                     | 0.40              |
| 36:N:119:LYS:HE2  | 36:N:119:LYS:HB3  | 1.92                     | 0.40              |
| 38:P:21:HIS:CD2   | 50:3:707:U:H4'    | 2.56                     | 0.40              |
| 38:P:127:ARG:HG3  | 48:Z:34:ARG:HH21  | 1.86                     | 0.40              |
| 39:Q:6:LEU:HD13   | 44:V:33:TYR:CE1   | 2.56                     | 0.40              |
| 39:Q:109:ARG:HH11 | 39:Q:109:ARG:HA   | 1.87                     | 0.40              |
| 46:X:77:ARG:CZ    | 50:3:1222:G:H5''  | 2.50                     | 0.40              |
| 50:3:131:A:H2'    | 50:3:132:C:C6     | 2.56                     | 0.40              |
| 50:3:168:G:O2'    | 50:3:169:C:H5'    | 2.22                     | 0.40              |
| 50:3:225:C:H2'    | 50:3:226:G:C4'    | 2.51                     | 0.40              |
| 50:3:948:C:H2'    | 50:3:949:A:H8     | 1.87                     | 0.40              |
| 50:3:1411:C:H2'   | 50:3:1412:C:C6    | 2.56                     | 0.40              |
| 51:1:20:C:H2'     | 51:1:21:A:C8      | 2.56                     | 0.40              |
| 51:1:845:A:H3'    | 51:1:845:A:N3     | 2.36                     | 0.40              |
| 51:1:1171:G:H2'   | 51:1:1172:C:H4'   | 2.04                     | 0.40              |
| 51:1:1229:C:H2'   | 51:1:1230:A:C8    | 2.56                     | 0.40              |
| 51:1:1751:U:H2'   | 51:1:1752:C:H5'   | 2.02                     | 0.40              |
| 51:1:1890:A:H2'   | 51:1:1891:G:O4'   | 2.21                     | 0.40              |
| 51:1:2315:G:O2'   | 51:1:2316:G:H5'   | 2.21                     | 0.40              |
| 51:1:2737:G:H2'   | 51:1:2738:A:C8    | 2.57                     | 0.40              |
| 55:8:4:ILE:N      | 55:8:4:ILE:CD1    | 2.78                     | 0.40              |
| 1:b:43:ASN:HD21   | 1:b:45:ASN:HB2    | 1.86                     | 0.40              |
| 1:b:55:GLY:O      | 1:b:214:GLY:HA2   | 2.20                     | 0.40              |
| 1:b:124:LYS:HD3   | 1:b:124:LYS:C     | 2.46                     | 0.40              |
| 1:b:242:HIS:O     | 1:b:244:VAL:HG23  | 2.22                     | 0.40              |
| 2:c:32:ASN:HB2    | 2:c:96:ILE:HB     | 2.02                     | 0.40              |
| 4:e:79:ARG:CG     | 4:e:80:GLN:H      | 2.33                     | 0.40              |
| 8:k:71:ARG:C      | 8:k:73:ASP:H      | 2.28                     | 0.40              |
| 11:n:2:ARG:O      | 11:n:2:ARG:CD     | 2.69                     | 0.40              |
| 12:o:90:VAL:HG11  | 12:o:115:LEU:HD21 | 2.03                     | 0.40              |
| 14:q:82:LEU:HD22  | 14:q:87:VAL:HG21  | 2.04                     | 0.40              |
| 15:r:66:HIS:CE1   | 15:r:94:THR:HG23  | 2.57                     | 0.40              |
| 18:u:45:GLN:O     | 51:1:483:A:H4'    | 2.21                     | 0.40              |
| 19:v:3:THR:HA     | 19:v:62:THR:OG1   | 2.22                     | 0.40              |
| 29:G:39:ILE:H     | 29:G:39:ILE:CD1   | 2.29                     | 0.40              |
| 32:J:104:ILE:HD13 | 32:J:122:VAL:HB   | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 33:K:14:GLN:HA   | 33:K:17:GLN:HE21 | 1.87                     | 0.40              |
| 33:K:38:ARG:HD3  | 33:K:98:GLU:H    | 1.87                     | 0.40              |
| 34:L:3:ARG:HD2   | 50:3:932:C:OP1   | 2.21                     | 0.40              |
| 34:L:32:ASP:HB2  | 34:L:34:LYS:HG3  | 2.04                     | 0.40              |
| 35:M:89:ASP:OD1  | 35:M:89:ASP:N    | 2.54                     | 0.40              |
| 40:R:53:ASP:N    | 40:R:53:ASP:OD1  | 2.54                     | 0.40              |
| 41:S:83:VAL:O    | 41:S:87:ALA:N    | 2.51                     | 0.40              |
| 41:S:92:ILE:HA   | 41:S:93:PRO:HD3  | 1.85                     | 0.40              |
| 43:U:19:VAL:HG13 | 43:U:19:VAL:O    | 2.21                     | 0.40              |
| 50:3:921:U:H5''  | 50:3:1082:A:C5'  | 2.52                     | 0.40              |
| 51:1:577:G:H2'   | 51:1:578:G:C8    | 2.57                     | 0.40              |
| 51:1:717:C:C2'   | 51:1:718:A:H5'   | 2.51                     | 0.40              |
| 51:1:727:A:H2'   | 51:1:728:G:O4'   | 2.21                     | 0.40              |
| 51:1:818:G:C2'   | 51:1:819:A:H5''  | 2.52                     | 0.40              |
| 51:1:1259:G:H2'  | 51:1:1260:A:H8   | 1.87                     | 0.40              |
| 51:1:1299:G:O6   | 51:1:1639:C:H5'' | 2.21                     | 0.40              |
| 51:1:1432:G:H2'  | 51:1:1433:A:C8   | 2.57                     | 0.40              |
| 51:1:1443:U:H2'  | 51:1:1444:G:C8   | 2.57                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | b     | 269/273 (98%) | 223 (83%) | 44 (16%) | 2 (1%)   | 18          | 53 |
| 2   | c     | 207/209 (99%) | 183 (88%) | 22 (11%) | 2 (1%)   | 12          | 45 |
| 3   | d     | 199/201 (99%) | 162 (81%) | 34 (17%) | 3 (2%)   | 8           | 37 |
| 4   | e     | 175/179 (98%) | 132 (75%) | 40 (23%) | 3 (2%)   | 7           | 35 |
| 5   | f     | 174/177 (98%) | 152 (87%) | 21 (12%) | 1 (1%)   | 21          | 55 |
| 6   | g     | 147/149 (99%) | 121 (82%) | 22 (15%) | 4 (3%)   | 4           | 28 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 7   | j     | 140/142 (99%) | 130 (93%) | 9 (6%)   | 1 (1%)   | 18          | 53  |
| 8   | k     | 120/123 (98%) | 106 (88%) | 12 (10%) | 2 (2%)   | 7           | 35  |
| 9   | l     | 141/144 (98%) | 118 (84%) | 22 (16%) | 1 (1%)   | 18          | 53  |
| 10  | m     | 134/136 (98%) | 110 (82%) | 19 (14%) | 5 (4%)   | 2           | 22  |
| 11  | n     | 118/127 (93%) | 105 (89%) | 10 (8%)  | 3 (2%)   | 4           | 29  |
| 12  | o     | 114/117 (97%) | 108 (95%) | 5 (4%)   | 1 (1%)   | 14          | 47  |
| 13  | p     | 112/115 (97%) | 97 (87%)  | 13 (12%) | 2 (2%)   | 6           | 34  |
| 14  | q     | 115/118 (98%) | 112 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 15  | r     | 101/103 (98%) | 80 (79%)  | 18 (18%) | 3 (3%)   | 3           | 26  |
| 16  | s     | 108/110 (98%) | 99 (92%)  | 6 (6%)   | 3 (3%)   | 4           | 27  |
| 17  | t     | 91/100 (91%)  | 80 (88%)  | 10 (11%) | 1 (1%)   | 11          | 43  |
| 18  | u     | 100/104 (96%) | 80 (80%)  | 18 (18%) | 2 (2%)   | 6           | 32  |
| 19  | v     | 92/94 (98%)   | 81 (88%)  | 11 (12%) | 0        | 100         | 100 |
| 20  | w     | 73/85 (86%)   | 61 (84%)  | 11 (15%) | 1 (1%)   | 9           | 38  |
| 21  | x     | 75/78 (96%)   | 70 (93%)  | 4 (5%)   | 1 (1%)   | 9           | 40  |
| 22  | y     | 61/63 (97%)   | 58 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 23  | z     | 56/59 (95%)   | 51 (91%)  | 4 (7%)   | 1 (2%)   | 6           | 34  |
| 24  | B     | 54/57 (95%)   | 51 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 25  | C     | 48/55 (87%)   | 45 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 26  | D     | 44/46 (96%)   | 39 (89%)  | 3 (7%)   | 2 (4%)   | 2           | 19  |
| 27  | E     | 62/65 (95%)   | 55 (89%)  | 6 (10%)  | 1 (2%)   | 7           | 36  |
| 28  | F     | 36/38 (95%)   | 28 (78%)  | 7 (19%)  | 1 (3%)   | 4           | 27  |
| 29  | G     | 223/241 (92%) | 189 (85%) | 29 (13%) | 5 (2%)   | 5           | 31  |
| 30  | H     | 204/233 (88%) | 178 (87%) | 25 (12%) | 1 (0%)   | 24          | 59  |
| 31  | I     | 203/206 (98%) | 169 (83%) | 28 (14%) | 6 (3%)   | 3           | 26  |
| 32  | J     | 155/167 (93%) | 136 (88%) | 16 (10%) | 3 (2%)   | 6           | 33  |
| 33  | K     | 99/131 (76%)  | 81 (82%)  | 13 (13%) | 5 (5%)   | 1           | 17  |
| 34  | L     | 149/156 (96%) | 131 (88%) | 18 (12%) | 0        | 100         | 100 |
| 35  | M     | 127/130 (98%) | 110 (87%) | 15 (12%) | 2 (2%)   | 7           | 36  |
| 36  | N     | 125/130 (96%) | 104 (83%) | 17 (14%) | 4 (3%)   | 3           | 25  |
| 37  | O     | 96/103 (93%)  | 77 (80%)  | 17 (18%) | 2 (2%)   | 5           | 31  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 38  | P     | 114/129 (88%)   | 93 (82%)   | 21 (18%)  | 0        | 100         | 100 |
| 39  | Q     | 121/124 (98%)   | 100 (83%)  | 18 (15%)  | 3 (2%)   | 4           | 29  |
| 40  | R     | 112/118 (95%)   | 101 (90%)  | 10 (9%)   | 1 (1%)   | 14          | 47  |
| 41  | S     | 98/101 (97%)    | 83 (85%)   | 14 (14%)  | 1 (1%)   | 12          | 45  |
| 42  | T     | 86/89 (97%)     | 75 (87%)   | 9 (10%)   | 2 (2%)   | 5           | 30  |
| 43  | U     | 80/82 (98%)     | 72 (90%)   | 8 (10%)   | 0        | 100         | 100 |
| 44  | V     | 78/84 (93%)     | 67 (86%)   | 10 (13%)  | 1 (1%)   | 9           | 40  |
| 45  | W     | 63/75 (84%)     | 56 (89%)   | 7 (11%)   | 0        | 100         | 100 |
| 46  | X     | 77/92 (84%)     | 66 (86%)   | 10 (13%)  | 1 (1%)   | 9           | 40  |
| 47  | Y     | 83/87 (95%)     | 75 (90%)   | 7 (8%)    | 1 (1%)   | 10          | 41  |
| 48  | Z     | 63/71 (89%)     | 42 (67%)   | 16 (25%)  | 5 (8%)   | 1           | 11  |
| 49  | a     | 130/234 (56%)   | 117 (90%)  | 13 (10%)  | 0        | 100         | 100 |
| 55  | 8     | 359/371 (97%)   | 313 (87%)  | 42 (12%)  | 4 (1%)   | 11          | 43  |
| All | All   | 6011/6421 (94%) | 5172 (86%) | 746 (12%) | 93 (2%)  | 11          | 37  |

All (93) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | d     | 9   | GLN  |
| 3   | d     | 83  | VAL  |
| 6   | g     | 9   | VAL  |
| 6   | g     | 11  | ASN  |
| 15  | r     | 55  | ASP  |
| 15  | r     | 80  | ARG  |
| 18  | u     | 99  | SER  |
| 27  | E     | 31  | ILE  |
| 32  | J     | 93  | VAL  |
| 33  | K     | 56  | LYS  |
| 33  | K     | 92  | THR  |
| 36  | N     | 57  | VAL  |
| 39  | Q     | 77  | SER  |
| 40  | R     | 11  | HIS  |
| 42  | T     | 46  | LYS  |
| 47  | Y     | 68  | LYS  |
| 48  | Z     | 8   | ASN  |
| 48  | Z     | 12  | ASP  |
| 48  | Z     | 65  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 111 | ALA  |
| 3   | d     | 6   | LYS  |
| 4   | e     | 81  | GLY  |
| 6   | g     | 10  | ALA  |
| 7   | j     | 72  | LYS  |
| 10  | m     | 28  | PHE  |
| 10  | m     | 59  | ARG  |
| 10  | m     | 70  | ASP  |
| 17  | t     | 52  | GLU  |
| 18  | u     | 6   | ARG  |
| 20  | w     | 80  | ALA  |
| 29  | G     | 15  | PHE  |
| 29  | G     | 99  | MET  |
| 29  | G     | 129 | THR  |
| 32  | J     | 157 | GLY  |
| 33  | K     | 55  | HIS  |
| 36  | N     | 90  | ASP  |
| 42  | T     | 45  | HIS  |
| 46  | X     | 67  | GLY  |
| 55  | 8     | 211 | GLY  |
| 55  | 8     | 230 | ILE  |
| 4   | e     | 138 | PRO  |
| 6   | g     | 15  | LEU  |
| 12  | o     | 100 | HIS  |
| 13  | p     | 64  | SER  |
| 15  | r     | 58  | VAL  |
| 21  | x     | 2   | ARG  |
| 26  | D     | 4   | THR  |
| 31  | I     | 125 | ASN  |
| 32  | J     | 23  | THR  |
| 36  | N     | 102 | PHE  |
| 36  | N     | 120 | ALA  |
| 44  | V     | 17  | GLU  |
| 2   | c     | 150 | GLN  |
| 8   | k     | 72  | PRO  |
| 11  | n     | 71  | ARG  |
| 11  | n     | 80  | PHE  |
| 16  | s     | 40  | ASN  |
| 16  | s     | 64  | ALA  |
| 26  | D     | 44  | VAL  |
| 28  | F     | 34  | LYS  |
| 29  | G     | 94  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | H     | 156 | LEU  |
| 33  | K     | 33  | GLU  |
| 35  | M     | 67  | GLY  |
| 48  | Z     | 25  | ALA  |
| 4   | e     | 174 | PHE  |
| 8   | k     | 89  | ASN  |
| 10  | m     | 5   | LYS  |
| 10  | m     | 6   | ARG  |
| 11  | n     | 118 | ARG  |
| 13  | p     | 2   | ASN  |
| 23  | z     | 51  | SER  |
| 31  | I     | 32  | LYS  |
| 31  | I     | 47  | LEU  |
| 39  | Q     | 33  | CYS  |
| 16  | s     | 65  | ASP  |
| 31  | I     | 20  | LEU  |
| 35  | M     | 5   | PRO  |
| 39  | Q     | 107 | LYS  |
| 48  | Z     | 24  | LYS  |
| 2   | c     | 10  | GLY  |
| 9   | l     | 53  | GLY  |
| 31  | I     | 37  | PRO  |
| 37  | O     | 67  | ILE  |
| 1   | b     | 125 | PRO  |
| 29  | G     | 179 | GLY  |
| 33  | K     | 18  | VAL  |
| 55  | 8     | 269 | GLY  |
| 55  | 8     | 318 | GLY  |
| 31  | I     | 23  | GLY  |
| 37  | O     | 42  | LEU  |
| 41  | S     | 93  | PRO  |
| 5   | f     | 125 | PRO  |

### 5.3.2 Protein sidechains [i](#)

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     | 216/218 (99%)  | 215 (100%) | 1 (0%)   | 81          | 82  |
| 2   | c     | 164/164 (100%) | 164 (100%) | 0        | 100         | 100 |
| 3   | d     | 165/165 (100%) | 163 (99%)  | 2 (1%)   | 63          | 72  |
| 4   | e     | 148/150 (99%)  | 147 (99%)  | 1 (1%)   | 76          | 78  |
| 5   | f     | 137/138 (99%)  | 136 (99%)  | 1 (1%)   | 76          | 78  |
| 6   | g     | 114/114 (100%) | 113 (99%)  | 1 (1%)   | 70          | 75  |
| 7   | j     | 116/116 (100%) | 116 (100%) | 0        | 100         | 100 |
| 8   | k     | 103/104 (99%)  | 103 (100%) | 0        | 100         | 100 |
| 9   | l     | 102/103 (99%)  | 101 (99%)  | 1 (1%)   | 68          | 75  |
| 10  | m     | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 11  | n     | 100/104 (96%)  | 100 (100%) | 0        | 100         | 100 |
| 12  | o     | 86/87 (99%)    | 85 (99%)   | 1 (1%)   | 63          | 72  |
| 13  | p     | 99/100 (99%)   | 94 (95%)   | 5 (5%)   | 21          | 46  |
| 14  | q     | 89/90 (99%)    | 89 (100%)  | 0        | 100         | 100 |
| 15  | r     | 84/84 (100%)   | 84 (100%)  | 0        | 100         | 100 |
| 16  | s     | 93/93 (100%)   | 93 (100%)  | 0        | 100         | 100 |
| 17  | t     | 80/84 (95%)    | 79 (99%)   | 1 (1%)   | 61          | 71  |
| 18  | u     | 83/85 (98%)    | 83 (100%)  | 0        | 100         | 100 |
| 19  | v     | 78/78 (100%)   | 78 (100%)  | 0        | 100         | 100 |
| 20  | w     | 57/63 (90%)    | 57 (100%)  | 0        | 100         | 100 |
| 21  | x     | 67/68 (98%)    | 67 (100%)  | 0        | 100         | 100 |
| 22  | y     | 55/55 (100%)   | 55 (100%)  | 0        | 100         | 100 |
| 23  | z     | 48/49 (98%)    | 48 (100%)  | 0        | 100         | 100 |
| 24  | B     | 47/48 (98%)    | 47 (100%)  | 0        | 100         | 100 |
| 25  | C     | 45/49 (92%)    | 45 (100%)  | 0        | 100         | 100 |
| 26  | D     | 38/38 (100%)   | 38 (100%)  | 0        | 100         | 100 |
| 27  | E     | 51/52 (98%)    | 51 (100%)  | 0        | 100         | 100 |
| 28  | F     | 34/34 (100%)   | 34 (100%)  | 0        | 100         | 100 |
| 29  | G     | 186/199 (94%)  | 186 (100%) | 0        | 100         | 100 |
| 30  | H     | 170/190 (90%)  | 170 (100%) | 0        | 100         | 100 |
| 31  | I     | 172/173 (99%)  | 169 (98%)  | 3 (2%)   | 53          | 68  |
| 32  | J     | 119/126 (94%)  | 117 (98%)  | 2 (2%)   | 53          | 68  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 33  | K     | 88/112 (79%)    | 86 (98%)   | 2 (2%)   | 44          | 63  |
| 34  | L     | 124/129 (96%)   | 123 (99%)  | 1 (1%)   | 73          | 77  |
| 35  | M     | 104/105 (99%)   | 103 (99%)  | 1 (1%)   | 68          | 75  |
| 36  | N     | 105/107 (98%)   | 105 (100%) | 0        | 100         | 100 |
| 37  | O     | 86/90 (96%)     | 84 (98%)   | 2 (2%)   | 44          | 63  |
| 38  | P     | 89/99 (90%)     | 88 (99%)   | 1 (1%)   | 65          | 74  |
| 39  | Q     | 103/104 (99%)   | 103 (100%) | 0        | 100         | 100 |
| 40  | R     | 92/96 (96%)     | 91 (99%)   | 1 (1%)   | 65          | 74  |
| 41  | S     | 83/84 (99%)     | 82 (99%)   | 1 (1%)   | 63          | 72  |
| 42  | T     | 76/77 (99%)     | 76 (100%)  | 0        | 100         | 100 |
| 43  | U     | 65/65 (100%)    | 65 (100%)  | 0        | 100         | 100 |
| 44  | V     | 74/78 (95%)     | 73 (99%)   | 1 (1%)   | 59          | 71  |
| 45  | W     | 56/65 (86%)     | 56 (100%)  | 0        | 100         | 100 |
| 46  | X     | 70/79 (89%)     | 69 (99%)   | 1 (1%)   | 59          | 71  |
| 47  | Y     | 65/66 (98%)     | 65 (100%)  | 0        | 100         | 100 |
| 48  | Z     | 55/61 (90%)     | 55 (100%)  | 0        | 100         | 100 |
| 49  | a     | 110/181 (61%)   | 108 (98%)  | 2 (2%)   | 51          | 67  |
| 55  | 8     | 307/317 (97%)   | 304 (99%)  | 3 (1%)   | 68          | 75  |
| All | All   | 5007/5245 (96%) | 4972 (99%) | 35 (1%)  | 73          | 78  |

All (35) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 225 | ASN  |
| 3   | d     | 152 | GLU  |
| 3   | d     | 184 | ASP  |
| 4   | e     | 176 | PHE  |
| 5   | f     | 102 | ILE  |
| 6   | g     | 127 | GLU  |
| 9   | l     | 92  | LEU  |
| 12  | o     | 100 | HIS  |
| 13  | p     | 4   | ILE  |
| 13  | p     | 47  | ILE  |
| 13  | p     | 83  | ILE  |
| 13  | p     | 109 | ILE  |
| 13  | p     | 113 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | t     | 87  | LEU  |
| 31  | I     | 33  | ILE  |
| 31  | I     | 127 | ARG  |
| 31  | I     | 131 | ILE  |
| 32  | J     | 10  | LEU  |
| 32  | J     | 55  | VAL  |
| 33  | K     | 55  | HIS  |
| 33  | K     | 94  | HIS  |
| 34  | L     | 84  | TYR  |
| 35  | M     | 90  | GLU  |
| 37  | O     | 76  | ILE  |
| 37  | O     | 97  | ASP  |
| 38  | P     | 54  | SER  |
| 40  | R     | 85  | TYR  |
| 41  | S     | 78  | LEU  |
| 44  | V     | 37  | ILE  |
| 46  | X     | 14  | LEU  |
| 49  | a     | 22  | ASP  |
| 49  | a     | 172 | HIS  |
| 55  | 8     | 4   | ILE  |
| 55  | 8     | 281 | HIS  |
| 55  | 8     | 349 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 36  | ASN  |
| 1   | b     | 43  | ASN  |
| 1   | b     | 44  | ASN  |
| 1   | b     | 85  | ASN  |
| 1   | b     | 89  | ASN  |
| 1   | b     | 116 | GLN  |
| 1   | b     | 196 | ASN  |
| 1   | b     | 199 | HIS  |
| 1   | b     | 225 | ASN  |
| 1   | b     | 231 | HIS  |
| 1   | b     | 238 | ASN  |
| 2   | c     | 32  | ASN  |
| 2   | c     | 49  | GLN  |
| 2   | c     | 173 | GLN  |
| 3   | d     | 30  | GLN  |
| 3   | d     | 136 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | e     | 20  | ASN  |
| 4   | e     | 51  | ASN  |
| 4   | e     | 80  | GLN  |
| 4   | e     | 134 | GLN  |
| 5   | f     | 115 | GLN  |
| 5   | f     | 142 | GLN  |
| 6   | g     | 11  | ASN  |
| 6   | g     | 20  | ASN  |
| 6   | g     | 43  | ASN  |
| 6   | g     | 66  | ASN  |
| 7   | j     | 40  | HIS  |
| 7   | j     | 58  | ASN  |
| 7   | j     | 128 | ASN  |
| 7   | j     | 136 | GLN  |
| 8   | k     | 3   | GLN  |
| 8   | k     | 5   | GLN  |
| 8   | k     | 90  | ASN  |
| 9   | l     | 38  | GLN  |
| 9   | l     | 54  | GLN  |
| 9   | l     | 104 | GLN  |
| 10  | m     | 3   | GLN  |
| 11  | n     | 9   | GLN  |
| 11  | n     | 62  | ASN  |
| 13  | p     | 2   | ASN  |
| 13  | p     | 40  | GLN  |
| 13  | p     | 65  | ASN  |
| 14  | q     | 36  | GLN  |
| 14  | q     | 43  | GLN  |
| 15  | r     | 11  | GLN  |
| 15  | r     | 18  | GLN  |
| 15  | r     | 87  | GLN  |
| 16  | s     | 7   | HIS  |
| 16  | s     | 9   | HIS  |
| 16  | s     | 40  | ASN  |
| 16  | s     | 57  | ASN  |
| 17  | t     | 15  | HIS  |
| 17  | t     | 28  | ASN  |
| 17  | t     | 48  | GLN  |
| 18  | u     | 68  | ASN  |
| 20  | w     | 42  | HIS  |
| 20  | w     | 53  | HIS  |
| 21  | x     | 15  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | x     | 31  | ASN  |
| 21  | x     | 33  | HIS  |
| 22  | y     | 27  | ASN  |
| 22  | y     | 31  | GLN  |
| 22  | y     | 36  | GLN  |
| 22  | y     | 45  | GLN  |
| 23  | z     | 8   | GLN  |
| 24  | B     | 3   | GLN  |
| 25  | C     | 25  | ASN  |
| 27  | E     | 30  | HIS  |
| 28  | F     | 35  | GLN  |
| 29  | G     | 18  | GLN  |
| 29  | G     | 50  | ASN  |
| 29  | G     | 57  | ASN  |
| 29  | G     | 108 | GLN  |
| 29  | G     | 119 | GLN  |
| 29  | G     | 167 | HIS  |
| 29  | G     | 189 | ASN  |
| 30  | H     | 2   | GLN  |
| 30  | H     | 7   | ASN  |
| 30  | H     | 139 | ASN  |
| 30  | H     | 184 | ASN  |
| 31  | I     | 40  | HIS  |
| 31  | I     | 58  | GLN  |
| 31  | I     | 88  | ASN  |
| 31  | I     | 99  | ASN  |
| 31  | I     | 135 | GLN  |
| 31  | I     | 163 | GLN  |
| 31  | I     | 195 | ASN  |
| 31  | I     | 197 | HIS  |
| 32  | J     | 11  | GLN  |
| 32  | J     | 72  | ASN  |
| 32  | J     | 131 | ASN  |
| 32  | J     | 134 | ASN  |
| 33  | K     | 17  | GLN  |
| 33  | K     | 37  | HIS  |
| 34  | L     | 27  | ASN  |
| 34  | L     | 121 | ASN  |
| 34  | L     | 141 | HIS  |
| 35  | M     | 3   | GLN  |
| 35  | M     | 15  | ASN  |
| 35  | M     | 17  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | M     | 20  | ASN  |
| 35  | M     | 37  | ASN  |
| 36  | N     | 4   | GLN  |
| 36  | N     | 74  | GLN  |
| 37  | O     | 15  | HIS  |
| 37  | O     | 70  | HIS  |
| 37  | O     | 99  | GLN  |
| 38  | P     | 21  | HIS  |
| 38  | P     | 23  | HIS  |
| 38  | P     | 28  | ASN  |
| 38  | P     | 118 | ASN  |
| 39  | Q     | 4   | ASN  |
| 39  | Q     | 5   | GLN  |
| 39  | Q     | 72  | ASN  |
| 40  | R     | 11  | HIS  |
| 42  | T     | 27  | GLN  |
| 42  | T     | 49  | HIS  |
| 42  | T     | 79  | GLN  |
| 43  | U     | 29  | ASN  |
| 45  | W     | 30  | ASN  |
| 46  | X     | 13  | HIS  |
| 46  | X     | 55  | GLN  |
| 47  | Y     | 2   | ASN  |
| 47  | Y     | 12  | GLN  |
| 47  | Y     | 20  | ASN  |
| 47  | Y     | 51  | ASN  |
| 47  | Y     | 69  | ASN  |
| 47  | Y     | 74  | HIS  |
| 47  | Y     | 81  | GLN  |
| 55  | 8     | 5   | ASN  |
| 55  | 8     | 38  | ASN  |
| 55  | 8     | 75  | GLN  |
| 55  | 8     | 97  | ASN  |
| 55  | 8     | 252 | GLN  |
| 55  | 8     | 280 | GLN  |
| 55  | 8     | 281 | HIS  |
| 55  | 8     | 301 | GLN  |
| 55  | 8     | 304 | ASN  |
| 55  | 8     | 308 | GLN  |
| 55  | 8     | 344 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 50  | 3     | 1538/1539 (99%) | 134 (8%)          | 2 (0%)          |
| 51  | 1     | 2902/2903 (99%) | 377 (12%)         | 4 (0%)          |
| 52  | 2     | 119/120 (99%)   | 9 (7%)            | 1 (0%)          |
| 53  | 5     | 72/77 (93%)     | 7 (9%)            | 0               |
| 54  | 4     | 19/27 (70%)     | 4 (21%)           | 0               |
| All | All   | 4650/4666 (99%) | 531 (11%)         | 7 (0%)          |

All (531) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | 3     | 9   | G    |
| 50  | 3     | 31  | G    |
| 50  | 3     | 32  | A    |
| 50  | 3     | 39  | G    |
| 50  | 3     | 48  | C    |
| 50  | 3     | 51  | A    |
| 50  | 3     | 71  | A    |
| 50  | 3     | 82  | G    |
| 50  | 3     | 85  | U    |
| 50  | 3     | 94  | G    |
| 50  | 3     | 100 | G    |
| 50  | 3     | 144 | G    |
| 50  | 3     | 168 | G    |
| 50  | 3     | 183 | C    |
| 50  | 3     | 184 | G    |
| 50  | 3     | 197 | A    |
| 50  | 3     | 210 | C    |
| 50  | 3     | 226 | G    |
| 50  | 3     | 247 | G    |
| 50  | 3     | 251 | G    |
| 50  | 3     | 266 | G    |
| 50  | 3     | 267 | C    |
| 50  | 3     | 280 | C    |
| 50  | 3     | 281 | G    |
| 50  | 3     | 289 | G    |
| 50  | 3     | 345 | C    |
| 50  | 3     | 352 | C    |
| 50  | 3     | 367 | U    |
| 50  | 3     | 372 | C    |
| 50  | 3     | 373 | A    |
| 50  | 3     | 411 | A    |
| 50  | 3     | 413 | G    |
| 50  | 3     | 422 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | 3     | 429 | U    |
| 50  | 3     | 467 | U    |
| 50  | 3     | 485 | U    |
| 50  | 3     | 486 | U    |
| 50  | 3     | 495 | A    |
| 50  | 3     | 497 | G    |
| 50  | 3     | 531 | U    |
| 50  | 3     | 532 | A    |
| 50  | 3     | 536 | C    |
| 50  | 3     | 547 | A    |
| 50  | 3     | 561 | U    |
| 50  | 3     | 564 | C    |
| 50  | 3     | 566 | G    |
| 50  | 3     | 572 | A    |
| 50  | 3     | 573 | A    |
| 50  | 3     | 575 | G    |
| 50  | 3     | 576 | C    |
| 50  | 3     | 577 | G    |
| 50  | 3     | 633 | G    |
| 50  | 3     | 653 | U    |
| 50  | 3     | 661 | G    |
| 50  | 3     | 665 | A    |
| 50  | 3     | 687 | A    |
| 50  | 3     | 688 | G    |
| 50  | 3     | 703 | G    |
| 50  | 3     | 724 | G    |
| 50  | 3     | 755 | G    |
| 50  | 3     | 777 | A    |
| 50  | 3     | 815 | A    |
| 50  | 3     | 817 | C    |
| 50  | 3     | 818 | G    |
| 50  | 3     | 819 | A    |
| 50  | 3     | 821 | G    |
| 50  | 3     | 843 | U    |
| 50  | 3     | 844 | G    |
| 50  | 3     | 845 | A    |
| 50  | 3     | 846 | G    |
| 50  | 3     | 847 | G    |
| 50  | 3     | 871 | U    |
| 50  | 3     | 872 | A    |
| 50  | 3     | 890 | G    |
| 50  | 3     | 926 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 50  | 3     | 934  | C    |
| 50  | 3     | 935  | A    |
| 50  | 3     | 960  | U    |
| 50  | 3     | 961  | U    |
| 50  | 3     | 966  | G    |
| 50  | 3     | 969  | A    |
| 50  | 3     | 975  | A    |
| 50  | 3     | 976  | G    |
| 50  | 3     | 977  | A    |
| 50  | 3     | 992  | U    |
| 50  | 3     | 993  | G    |
| 50  | 3     | 1004 | A    |
| 50  | 3     | 1028 | C    |
| 50  | 3     | 1030 | U    |
| 50  | 3     | 1033 | G    |
| 50  | 3     | 1034 | G    |
| 50  | 3     | 1094 | G    |
| 50  | 3     | 1101 | A    |
| 50  | 3     | 1135 | U    |
| 50  | 3     | 1136 | C    |
| 50  | 3     | 1137 | C    |
| 50  | 3     | 1138 | G    |
| 50  | 3     | 1139 | G    |
| 50  | 3     | 1159 | U    |
| 50  | 3     | 1168 | U    |
| 50  | 3     | 1182 | G    |
| 50  | 3     | 1191 | A    |
| 50  | 3     | 1196 | A    |
| 50  | 3     | 1198 | G    |
| 50  | 3     | 1202 | U    |
| 50  | 3     | 1212 | U    |
| 50  | 3     | 1213 | A    |
| 50  | 3     | 1225 | A    |
| 50  | 3     | 1238 | A    |
| 50  | 3     | 1240 | U    |
| 50  | 3     | 1241 | G    |
| 50  | 3     | 1275 | A    |
| 50  | 3     | 1278 | G    |
| 50  | 3     | 1280 | A    |
| 50  | 3     | 1282 | C    |
| 50  | 3     | 1286 | U    |
| 50  | 3     | 1287 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 50  | 3     | 1300 | G    |
| 50  | 3     | 1346 | A    |
| 50  | 3     | 1347 | G    |
| 50  | 3     | 1394 | A    |
| 50  | 3     | 1395 | C    |
| 50  | 3     | 1397 | C    |
| 50  | 3     | 1446 | A    |
| 50  | 3     | 1448 | C    |
| 50  | 3     | 1492 | A    |
| 50  | 3     | 1493 | A    |
| 50  | 3     | 1503 | A    |
| 50  | 3     | 1506 | U    |
| 50  | 3     | 1517 | G    |
| 50  | 3     | 1529 | G    |
| 50  | 3     | 1530 | G    |
| 50  | 3     | 1533 | C    |
| 50  | 3     | 1540 | U    |
| 51  | 1     | 10   | A    |
| 51  | 1     | 34   | U    |
| 51  | 1     | 35   | G    |
| 51  | 1     | 46   | G    |
| 51  | 1     | 50   | U    |
| 51  | 1     | 51   | G    |
| 51  | 1     | 61   | C    |
| 51  | 1     | 63   | A    |
| 51  | 1     | 71   | A    |
| 51  | 1     | 74   | A    |
| 51  | 1     | 75   | G    |
| 51  | 1     | 86   | G    |
| 51  | 1     | 114  | U    |
| 51  | 1     | 118  | A    |
| 51  | 1     | 120  | U    |
| 51  | 1     | 138  | U    |
| 51  | 1     | 140  | C    |
| 51  | 1     | 141  | G    |
| 51  | 1     | 162  | U    |
| 51  | 1     | 163  | C    |
| 51  | 1     | 181  | A    |
| 51  | 1     | 196  | A    |
| 51  | 1     | 216  | A    |
| 51  | 1     | 221  | A    |
| 51  | 1     | 222  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 1     | 228 | C    |
| 51  | 1     | 229 | C    |
| 51  | 1     | 248 | G    |
| 51  | 1     | 255 | A    |
| 51  | 1     | 265 | A    |
| 51  | 1     | 266 | G    |
| 51  | 1     | 276 | U    |
| 51  | 1     | 278 | A    |
| 51  | 1     | 281 | C    |
| 51  | 1     | 312 | G    |
| 51  | 1     | 323 | C    |
| 51  | 1     | 324 | A    |
| 51  | 1     | 329 | G    |
| 51  | 1     | 330 | A    |
| 51  | 1     | 362 | A    |
| 51  | 1     | 367 | G    |
| 51  | 1     | 371 | A    |
| 51  | 1     | 372 | G    |
| 51  | 1     | 386 | G    |
| 51  | 1     | 387 | U    |
| 51  | 1     | 391 | A    |
| 51  | 1     | 404 | A    |
| 51  | 1     | 406 | G    |
| 51  | 1     | 411 | G    |
| 51  | 1     | 412 | A    |
| 51  | 1     | 424 | G    |
| 51  | 1     | 451 | U    |
| 51  | 1     | 456 | C    |
| 51  | 1     | 457 | A    |
| 51  | 1     | 480 | A    |
| 51  | 1     | 481 | G    |
| 51  | 1     | 491 | G    |
| 51  | 1     | 504 | A    |
| 51  | 1     | 505 | A    |
| 51  | 1     | 508 | A    |
| 51  | 1     | 529 | A    |
| 51  | 1     | 530 | G    |
| 51  | 1     | 531 | C    |
| 51  | 1     | 532 | A    |
| 51  | 1     | 545 | U    |
| 51  | 1     | 548 | G    |
| 51  | 1     | 549 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 1     | 563 | A    |
| 51  | 1     | 571 | U    |
| 51  | 1     | 573 | U    |
| 51  | 1     | 574 | A    |
| 51  | 1     | 575 | A    |
| 51  | 1     | 588 | U    |
| 51  | 1     | 603 | A    |
| 51  | 1     | 616 | A    |
| 51  | 1     | 627 | A    |
| 51  | 1     | 637 | A    |
| 51  | 1     | 646 | U    |
| 51  | 1     | 647 | G    |
| 51  | 1     | 654 | A    |
| 51  | 1     | 669 | G    |
| 51  | 1     | 686 | U    |
| 51  | 1     | 687 | C    |
| 51  | 1     | 695 | G    |
| 51  | 1     | 730 | A    |
| 51  | 1     | 747 | C    |
| 51  | 1     | 752 | A    |
| 51  | 1     | 764 | A    |
| 51  | 1     | 776 | G    |
| 51  | 1     | 782 | A    |
| 51  | 1     | 783 | A    |
| 51  | 1     | 784 | G    |
| 51  | 1     | 785 | G    |
| 51  | 1     | 791 | C    |
| 51  | 1     | 792 | A    |
| 51  | 1     | 793 | A    |
| 51  | 1     | 805 | G    |
| 51  | 1     | 812 | C    |
| 51  | 1     | 819 | A    |
| 51  | 1     | 827 | U    |
| 51  | 1     | 828 | U    |
| 51  | 1     | 830 | G    |
| 51  | 1     | 831 | G    |
| 51  | 1     | 847 | U    |
| 51  | 1     | 859 | G    |
| 51  | 1     | 878 | A    |
| 51  | 1     | 886 | A    |
| 51  | 1     | 887 | U    |
| 51  | 1     | 891 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 893  | C    |
| 51  | 1     | 896  | A    |
| 51  | 1     | 910  | A    |
| 51  | 1     | 931  | U    |
| 51  | 1     | 932  | U    |
| 51  | 1     | 941  | A    |
| 51  | 1     | 946  | C    |
| 51  | 1     | 961  | C    |
| 51  | 1     | 962  | G    |
| 51  | 1     | 974  | G    |
| 51  | 1     | 983  | A    |
| 51  | 1     | 995  | C    |
| 51  | 1     | 996  | A    |
| 51  | 1     | 1009 | A    |
| 51  | 1     | 1012 | U    |
| 51  | 1     | 1013 | C    |
| 51  | 1     | 1021 | A    |
| 51  | 1     | 1022 | G    |
| 51  | 1     | 1025 | G    |
| 51  | 1     | 1026 | G    |
| 51  | 1     | 1033 | U    |
| 51  | 1     | 1046 | A    |
| 51  | 1     | 1062 | G    |
| 51  | 1     | 1064 | C    |
| 51  | 1     | 1065 | U    |
| 51  | 1     | 1066 | U    |
| 51  | 1     | 1070 | A    |
| 51  | 1     | 1071 | G    |
| 51  | 1     | 1075 | C    |
| 51  | 1     | 1078 | U    |
| 51  | 1     | 1079 | C    |
| 51  | 1     | 1084 | A    |
| 51  | 1     | 1087 | G    |
| 51  | 1     | 1088 | A    |
| 51  | 1     | 1089 | A    |
| 51  | 1     | 1094 | U    |
| 51  | 1     | 1104 | C    |
| 51  | 1     | 1111 | A    |
| 51  | 1     | 1131 | G    |
| 51  | 1     | 1132 | U    |
| 51  | 1     | 1135 | C    |
| 51  | 1     | 1143 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 1157 | G    |
| 51  | 1     | 1172 | C    |
| 51  | 1     | 1173 | U    |
| 51  | 1     | 1175 | A    |
| 51  | 1     | 1177 | G    |
| 51  | 1     | 1179 | G    |
| 51  | 1     | 1180 | U    |
| 51  | 1     | 1181 | U    |
| 51  | 1     | 1211 | C    |
| 51  | 1     | 1212 | G    |
| 51  | 1     | 1253 | A    |
| 51  | 1     | 1256 | G    |
| 51  | 1     | 1271 | G    |
| 51  | 1     | 1272 | A    |
| 51  | 1     | 1289 | C    |
| 51  | 1     | 1301 | A    |
| 51  | 1     | 1321 | A    |
| 51  | 1     | 1329 | U    |
| 51  | 1     | 1345 | C    |
| 51  | 1     | 1365 | A    |
| 51  | 1     | 1378 | A    |
| 51  | 1     | 1379 | U    |
| 51  | 1     | 1383 | A    |
| 51  | 1     | 1397 | U    |
| 51  | 1     | 1398 | C    |
| 51  | 1     | 1416 | G    |
| 51  | 1     | 1419 | A    |
| 51  | 1     | 1420 | A    |
| 51  | 1     | 1421 | G    |
| 51  | 1     | 1455 | G    |
| 51  | 1     | 1461 | C    |
| 51  | 1     | 1467 | U    |
| 51  | 1     | 1468 | U    |
| 51  | 1     | 1476 | U    |
| 51  | 1     | 1478 | G    |
| 51  | 1     | 1482 | G    |
| 51  | 1     | 1490 | A    |
| 51  | 1     | 1498 | C    |
| 51  | 1     | 1523 | U    |
| 51  | 1     | 1535 | A    |
| 51  | 1     | 1536 | C    |
| 51  | 1     | 1537 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 1555 | G    |
| 51  | 1     | 1559 | U    |
| 51  | 1     | 1569 | A    |
| 51  | 1     | 1581 | G    |
| 51  | 1     | 1585 | C    |
| 51  | 1     | 1607 | C    |
| 51  | 1     | 1608 | A    |
| 51  | 1     | 1611 | C    |
| 51  | 1     | 1616 | A    |
| 51  | 1     | 1647 | U    |
| 51  | 1     | 1648 | U    |
| 51  | 1     | 1674 | G    |
| 51  | 1     | 1703 | G    |
| 51  | 1     | 1715 | G    |
| 51  | 1     | 1723 | G    |
| 51  | 1     | 1730 | C    |
| 51  | 1     | 1731 | G    |
| 51  | 1     | 1733 | G    |
| 51  | 1     | 1738 | G    |
| 51  | 1     | 1739 | A    |
| 51  | 1     | 1740 | G    |
| 51  | 1     | 1743 | G    |
| 51  | 1     | 1752 | C    |
| 51  | 1     | 1758 | U    |
| 51  | 1     | 1764 | C    |
| 51  | 1     | 1773 | A    |
| 51  | 1     | 1800 | C    |
| 51  | 1     | 1801 | A    |
| 51  | 1     | 1802 | A    |
| 51  | 1     | 1808 | A    |
| 51  | 1     | 1816 | C    |
| 51  | 1     | 1821 | A    |
| 51  | 1     | 1829 | A    |
| 51  | 1     | 1848 | A    |
| 51  | 1     | 1866 | A    |
| 51  | 1     | 1870 | C    |
| 51  | 1     | 1884 | G    |
| 51  | 1     | 1901 | A    |
| 51  | 1     | 1906 | G    |
| 51  | 1     | 1913 | A    |
| 51  | 1     | 1915 | U    |
| 51  | 1     | 1930 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 1937 | A    |
| 51  | 1     | 1943 | U    |
| 51  | 1     | 1944 | U    |
| 51  | 1     | 1955 | U    |
| 51  | 1     | 1963 | U    |
| 51  | 1     | 1967 | C    |
| 51  | 1     | 1970 | A    |
| 51  | 1     | 1972 | G    |
| 51  | 1     | 1991 | U    |
| 51  | 1     | 1993 | U    |
| 51  | 1     | 1997 | C    |
| 51  | 1     | 2022 | U    |
| 51  | 1     | 2023 | C    |
| 51  | 1     | 2030 | A    |
| 51  | 1     | 2031 | A    |
| 51  | 1     | 2043 | C    |
| 51  | 1     | 2055 | C    |
| 51  | 1     | 2056 | G    |
| 51  | 1     | 2060 | A    |
| 51  | 1     | 2061 | G    |
| 51  | 1     | 2062 | A    |
| 51  | 1     | 2069 | G    |
| 51  | 1     | 2096 | C    |
| 51  | 1     | 2111 | U    |
| 51  | 1     | 2112 | G    |
| 51  | 1     | 2113 | U    |
| 51  | 1     | 2118 | U    |
| 51  | 1     | 2119 | A    |
| 51  | 1     | 2127 | G    |
| 51  | 1     | 2128 | G    |
| 51  | 1     | 2131 | U    |
| 51  | 1     | 2132 | U    |
| 51  | 1     | 2133 | G    |
| 51  | 1     | 2145 | C    |
| 51  | 1     | 2147 | A    |
| 51  | 1     | 2166 | U    |
| 51  | 1     | 2172 | U    |
| 51  | 1     | 2173 | A    |
| 51  | 1     | 2178 | C    |
| 51  | 1     | 2180 | U    |
| 51  | 1     | 2198 | A    |
| 51  | 1     | 2204 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 2213 | U    |
| 51  | 1     | 2225 | A    |
| 51  | 1     | 2238 | G    |
| 51  | 1     | 2239 | G    |
| 51  | 1     | 2243 | U    |
| 51  | 1     | 2245 | U    |
| 51  | 1     | 2247 | A    |
| 51  | 1     | 2250 | G    |
| 51  | 1     | 2255 | G    |
| 51  | 1     | 2259 | U    |
| 51  | 1     | 2278 | A    |
| 51  | 1     | 2283 | C    |
| 51  | 1     | 2286 | G    |
| 51  | 1     | 2297 | A    |
| 51  | 1     | 2300 | C    |
| 51  | 1     | 2305 | U    |
| 51  | 1     | 2306 | C    |
| 51  | 1     | 2307 | G    |
| 51  | 1     | 2308 | G    |
| 51  | 1     | 2309 | A    |
| 51  | 1     | 2310 | C    |
| 51  | 1     | 2311 | A    |
| 51  | 1     | 2312 | U    |
| 51  | 1     | 2314 | A    |
| 51  | 1     | 2317 | A    |
| 51  | 1     | 2325 | G    |
| 51  | 1     | 2327 | A    |
| 51  | 1     | 2334 | U    |
| 51  | 1     | 2335 | A    |
| 51  | 1     | 2361 | G    |
| 51  | 1     | 2382 | G    |
| 51  | 1     | 2383 | G    |
| 51  | 1     | 2385 | C    |
| 51  | 1     | 2390 | U    |
| 51  | 1     | 2391 | G    |
| 51  | 1     | 2402 | U    |
| 51  | 1     | 2424 | C    |
| 51  | 1     | 2425 | A    |
| 51  | 1     | 2426 | A    |
| 51  | 1     | 2427 | C    |
| 51  | 1     | 2429 | G    |
| 51  | 1     | 2430 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 2431 | U    |
| 51  | 1     | 2433 | A    |
| 51  | 1     | 2434 | A    |
| 51  | 1     | 2441 | U    |
| 51  | 1     | 2448 | A    |
| 51  | 1     | 2469 | A    |
| 51  | 1     | 2476 | A    |
| 51  | 1     | 2491 | U    |
| 51  | 1     | 2498 | C    |
| 51  | 1     | 2502 | G    |
| 51  | 1     | 2503 | A    |
| 51  | 1     | 2505 | G    |
| 51  | 1     | 2506 | U    |
| 51  | 1     | 2518 | A    |
| 51  | 1     | 2520 | C    |
| 51  | 1     | 2543 | G    |
| 51  | 1     | 2547 | A    |
| 51  | 1     | 2564 | A    |
| 51  | 1     | 2566 | A    |
| 51  | 1     | 2567 | G    |
| 51  | 1     | 2572 | A    |
| 51  | 1     | 2582 | G    |
| 51  | 1     | 2585 | U    |
| 51  | 1     | 2602 | A    |
| 51  | 1     | 2603 | G    |
| 51  | 1     | 2605 | U    |
| 51  | 1     | 2609 | U    |
| 51  | 1     | 2613 | U    |
| 51  | 1     | 2629 | U    |
| 51  | 1     | 2630 | G    |
| 51  | 1     | 2655 | G    |
| 51  | 1     | 2682 | A    |
| 51  | 1     | 2689 | U    |
| 51  | 1     | 2690 | U    |
| 51  | 1     | 2714 | G    |
| 51  | 1     | 2733 | A    |
| 51  | 1     | 2748 | A    |
| 51  | 1     | 2750 | A    |
| 51  | 1     | 2764 | A    |
| 51  | 1     | 2765 | A    |
| 51  | 1     | 2778 | A    |
| 51  | 1     | 2779 | U    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 51  | 1     | 2791  | G    |
| 51  | 1     | 2793  | C    |
| 51  | 1     | 2797  | U    |
| 51  | 1     | 2800  | A    |
| 51  | 1     | 2801  | G    |
| 51  | 1     | 2820  | A    |
| 51  | 1     | 2821  | A    |
| 51  | 1     | 2833  | U    |
| 51  | 1     | 2835  | A    |
| 51  | 1     | 2849  | U    |
| 51  | 1     | 2850  | A    |
| 51  | 1     | 2867  | G    |
| 51  | 1     | 2868  | A    |
| 51  | 1     | 2879  | A    |
| 51  | 1     | 2880  | C    |
| 51  | 1     | 2884  | U    |
| 52  | 2     | 4     | C    |
| 52  | 2     | 13    | G    |
| 52  | 2     | 24    | G    |
| 52  | 2     | 35    | C    |
| 52  | 2     | 44    | G    |
| 52  | 2     | 67    | G    |
| 52  | 2     | 89    | U    |
| 52  | 2     | 108   | A    |
| 52  | 2     | 109   | A    |
| 53  | 5     | 9     | G    |
| 53  | 5     | 17(A) | U    |
| 53  | 5     | 19    | G    |
| 53  | 5     | 48    | C    |
| 53  | 5     | 49    | G    |
| 53  | 5     | 59    | A    |
| 53  | 5     | 61    | C    |
| 54  | 4     | 12    | A    |
| 54  | 4     | 19    | U    |
| 54  | 4     | 22    | A    |
| 54  | 4     | 23    | A    |

All (7) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 50  | 3     | 1190 | G    |
| 50  | 3     | 1491 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 1     | 490  | C    |
| 51  | 1     | 1020 | A    |
| 51  | 1     | 1738 | G    |
| 51  | 1     | 2326 | C    |
| 52  | 2     | 88   | C    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

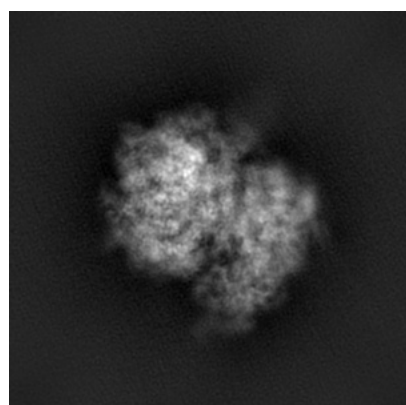
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20056. These allow visual inspection of the internal detail of the map and identification of artifacts.

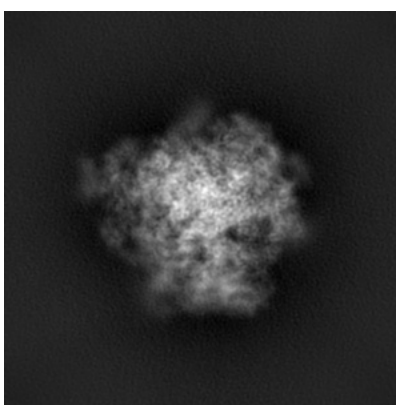
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

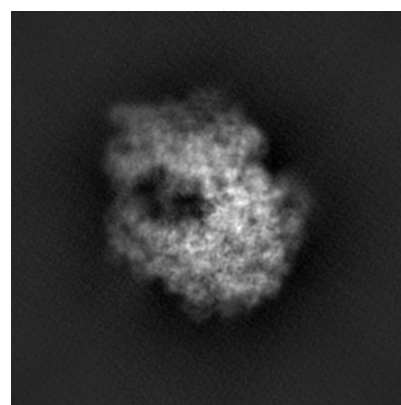
#### 6.1.1 Primary map



X



Y

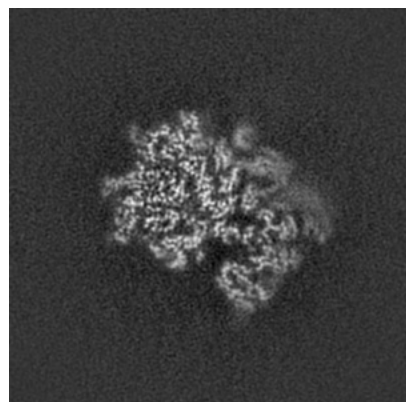


Z

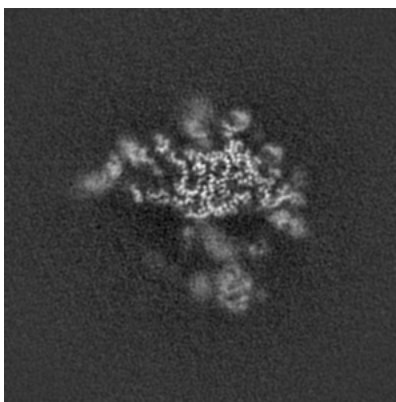
The images above show the map projected in three orthogonal directions.

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

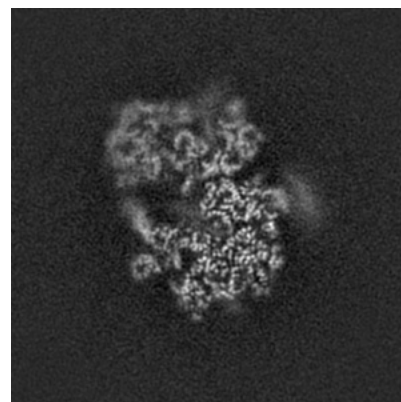
#### 6.2.1 Primary map



X Index: 156



Y Index: 156

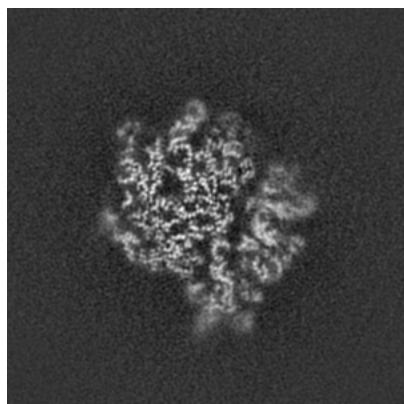


Z Index: 156

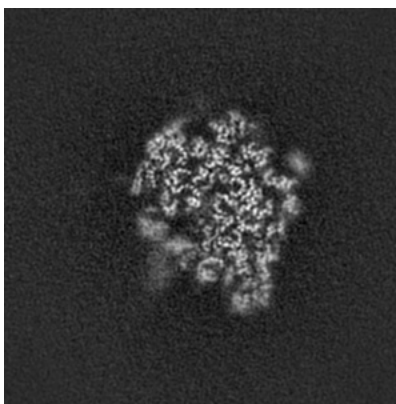
The images above show central slices of the map in three orthogonal directions.

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

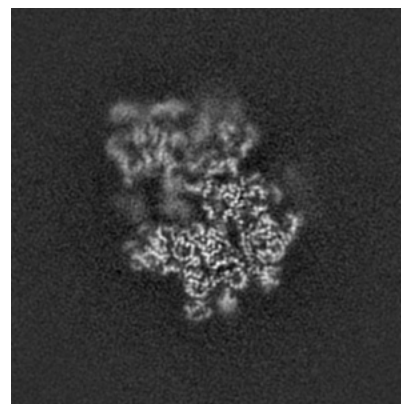
### 6.3.1 Primary map



X Index: 178



Y Index: 138

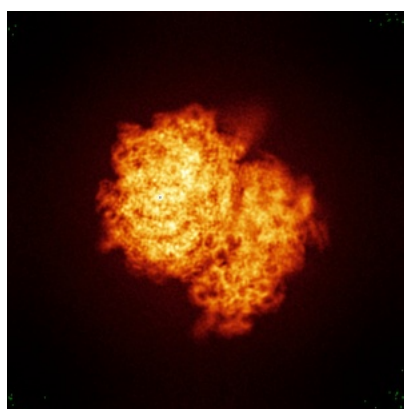


Z Index: 165

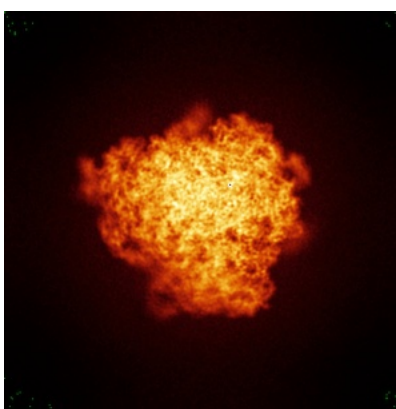
The images above show the largest variance slices of the map in three orthogonal directions.

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

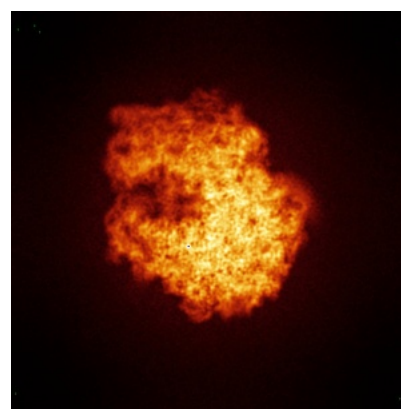
### 6.4.1 Primary map



X



Y



Z

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

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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

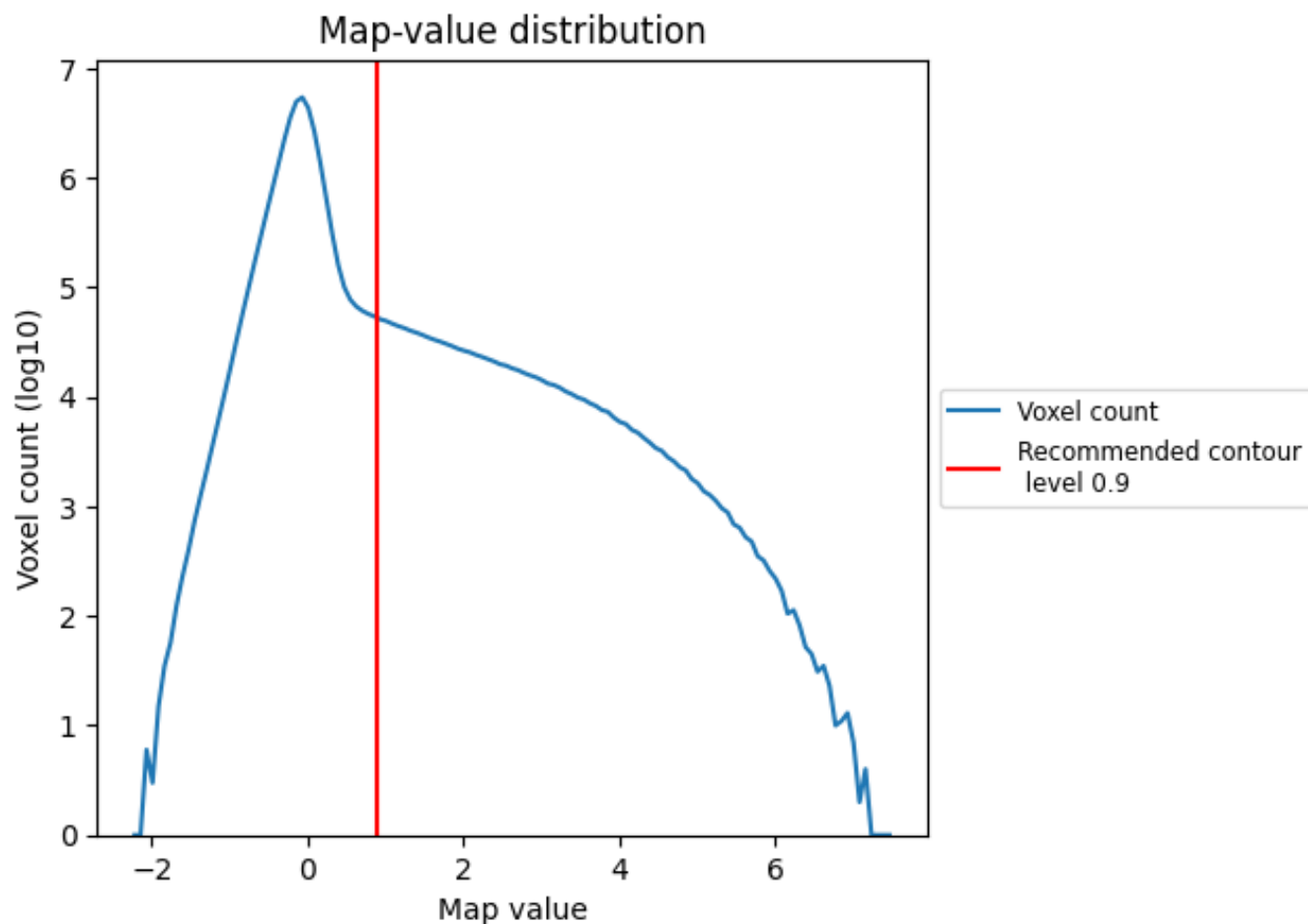
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

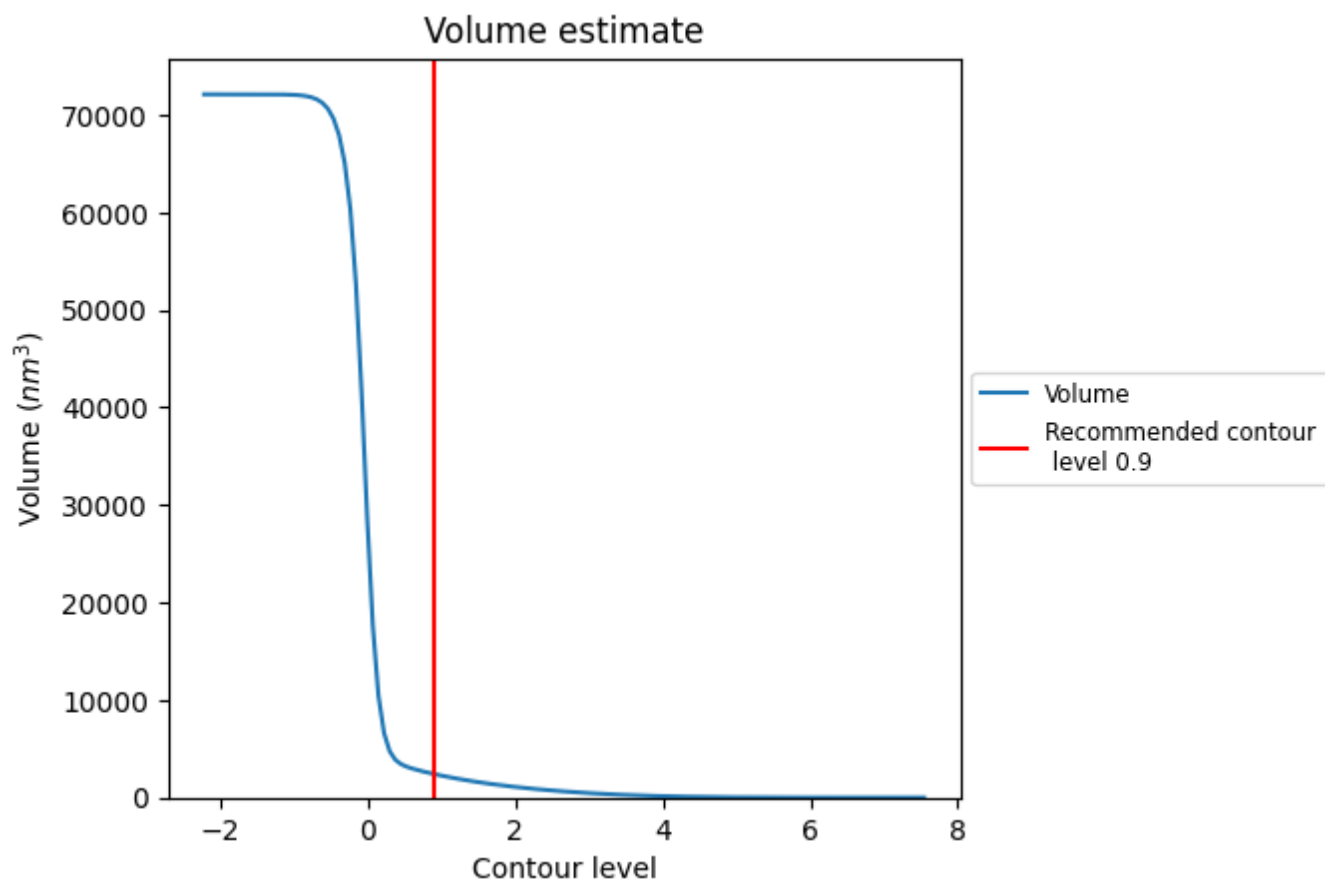
This section contains the results of statistical analysis of the map.

### 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.

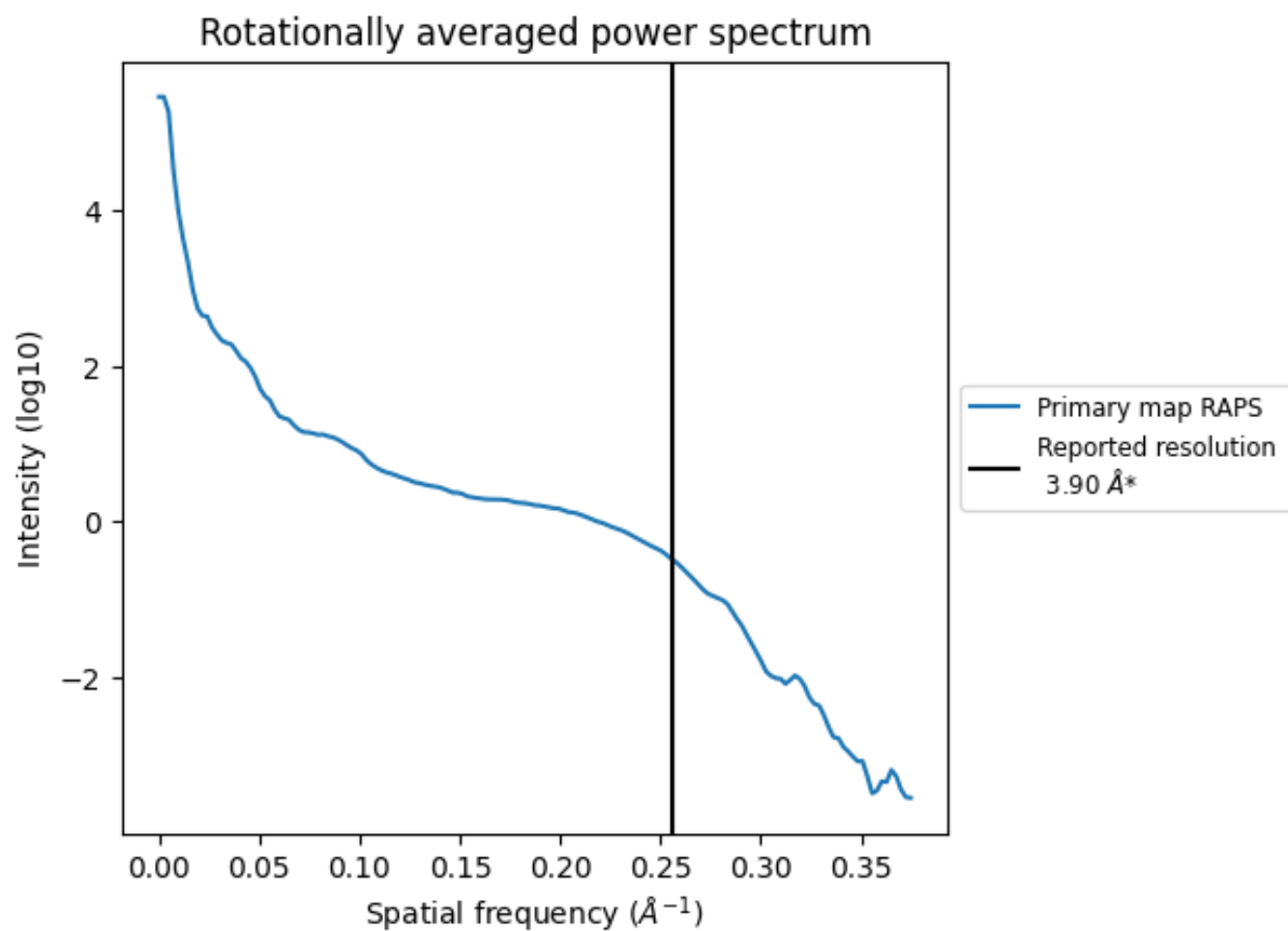
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2406 nm<sup>3</sup>; this corresponds to an approximate mass of 2174 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

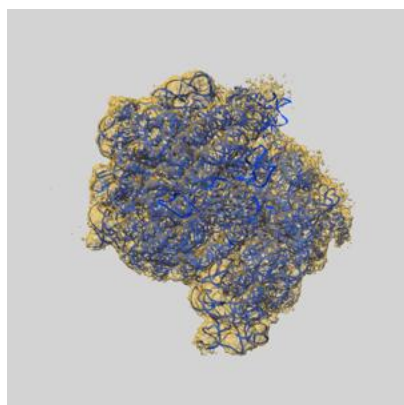
## 8 Fourier-Shell correlation

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

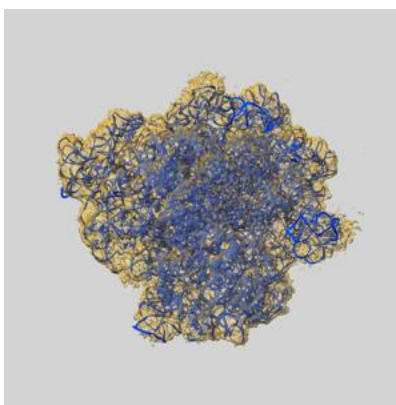
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20056 and PDB model 6OGF. Per-residue inclusion information can be found in section [3](#) on page [15](#).

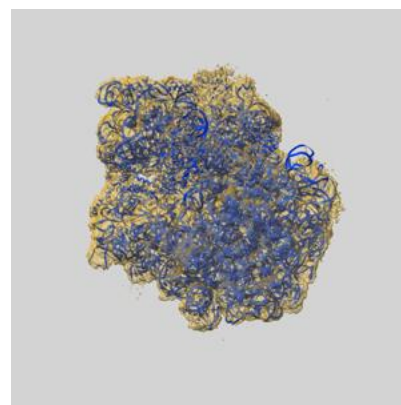
### 9.1 Map-model overlay [i](#)



X



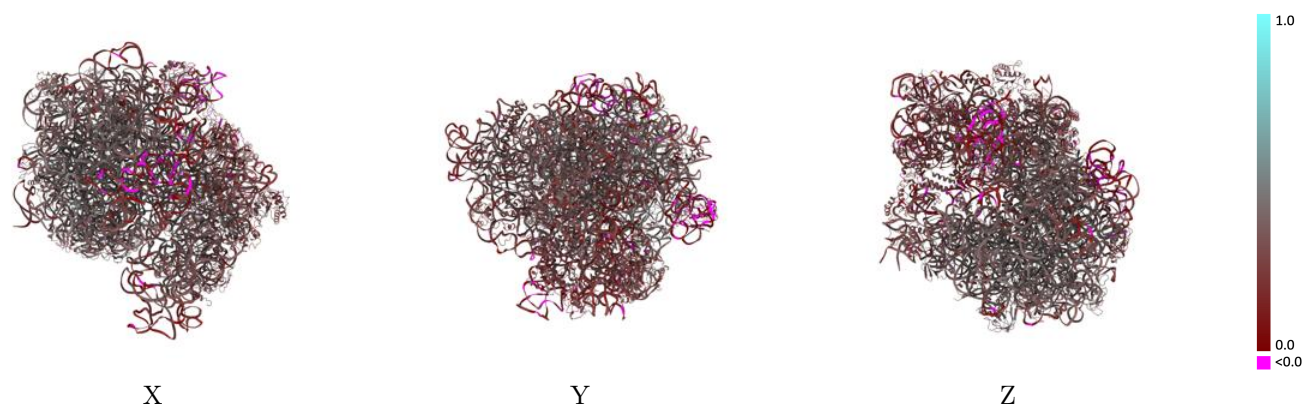
Y



Z

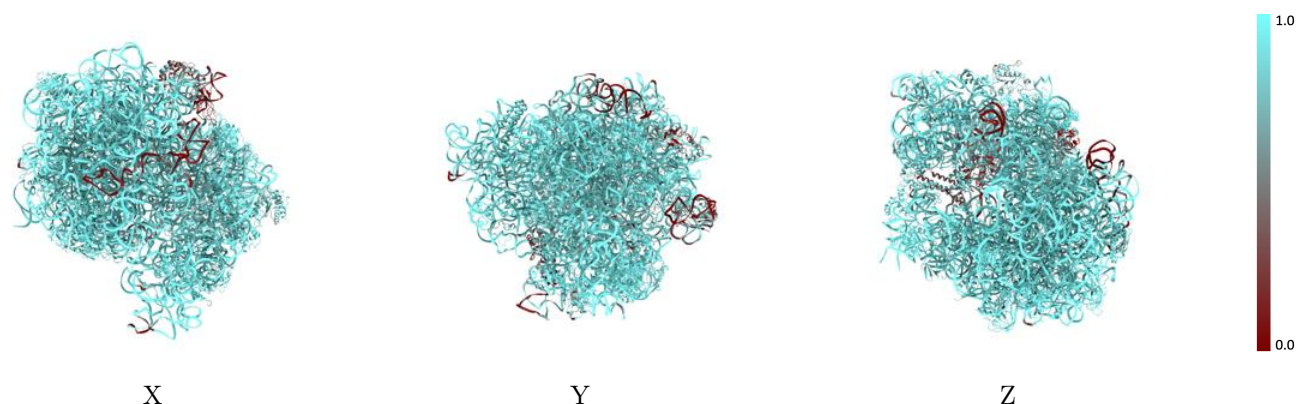
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



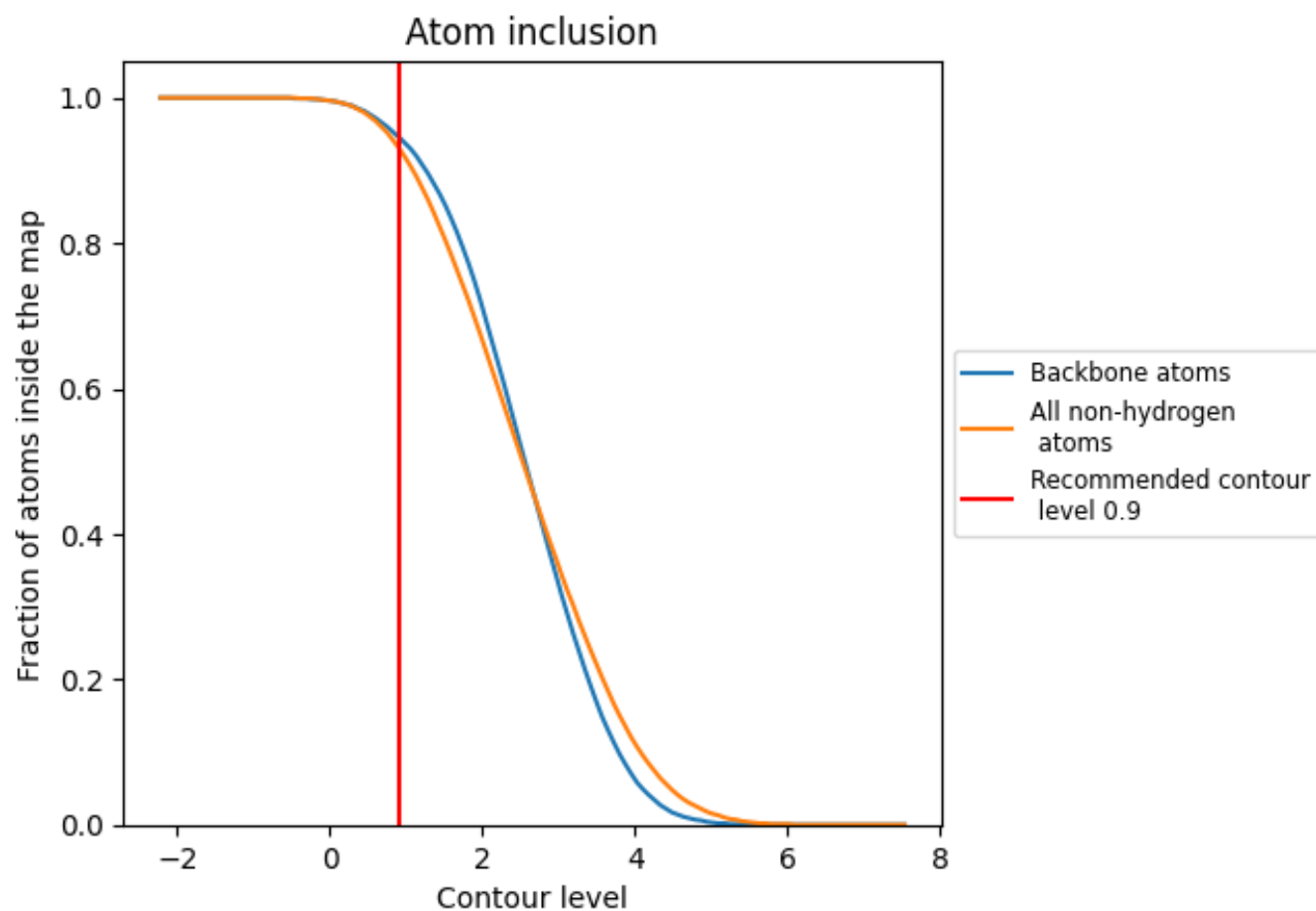
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.9).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.9) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9320   |  0.3280   |
| 1     |  0.9400   |  0.3440   |
| 2     |  0.9900   |  0.3090   |
| 3     |  0.9700   |  0.2980   |
| 4     |  0.9450   |  0.2110   |
| 5     |  0.7960   |  0.1450   |
| 8     |  0.6570   |  0.2920   |
| B     |  0.9600   |  0.4020   |
| C     |  0.9000   |  0.3730   |
| D     |  0.9520   |  0.4110   |
| E     |  0.9430   |  0.4160   |
| F     |  0.9420   |  0.3390   |
| G     |  0.8050   |  0.2850   |
| H     |  0.9090   |  0.2980   |
| I     |  0.8850  |  0.2800  |
| J     |  0.9480 |  0.3420 |
| K     |  0.9800 |  0.2690 |
| L     |  0.9300 |  0.2380 |
| M     |  0.9620 |  0.3250 |
| N     |  0.9560 |  0.2660 |
| O     |  0.8310 |  0.2570 |
| P     |  0.9750 |  0.2750 |
| Q     |  0.9340 |  0.3640 |
| R     |  0.9340 |  0.2510 |
| S     |  0.9410 |  0.2740 |
| T     |  0.9740 |  0.2750 |
| U     |  0.9440 |  0.3720 |
| V     |  0.9530 |  0.3550 |
| W     |  0.9510 |  0.2860 |
| X     |  0.9490 |  0.2570 |
| Y     |  0.9460 |  0.3160 |
| Z     |  0.8670 |  0.2450 |
| a     |  0.3680 |  0.2010 |
| b     |  0.9570 |  0.4090 |
| c     |  0.9680 |  0.4190 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| d     |  0.9470   |  0.3850   |
| e     |  0.9460   |  0.2600   |
| f     |  0.9040   |  0.3010   |
| g     |  0.3860   |  0.2880   |
| j     |  0.9660   |  0.4090   |
| k     |  0.9420   |  0.4210   |
| l     |  0.9630   |  0.4090   |
| m     |  0.9590   |  0.4010   |
| n     |  0.9710   |  0.4170   |
| o     |  0.9680   |  0.3410   |
| p     |  0.9550   |  0.4000   |
| q     |  0.9590   |  0.3940   |
| r     |  0.9590   |  0.4140   |
| s     |  0.9350   |  0.4190   |
| t     |  0.9430   |  0.3960   |
| u     |  0.9570   |  0.3800   |
| v     |  0.9590   |  0.3710   |
| w     |  0.9520  |  0.4140  |
| x     |  0.9550 |  0.3860 |
| y     |  0.9210 |  0.3230 |
| z     |  0.9340 |  0.4070 |