



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:18 AM UTC

PDB ID : 6WDH / pdb\_00006wdh  
EMDB ID : EMD-21636  
Title : Cryo-EM of elongating ribosome with EF-Tu\*GTP elucidates tRNA proof-reading (Non-cognate Structure IV-B1)  
Authors : Loveland, A.B.; Demo, G.; Korostelev, A.A.  
Deposited on : 2020-03-31  
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
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

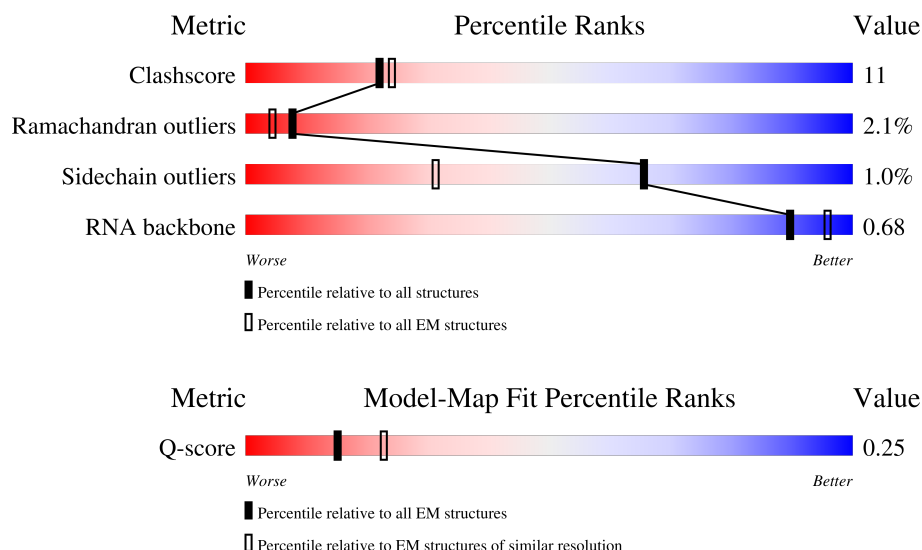
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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.



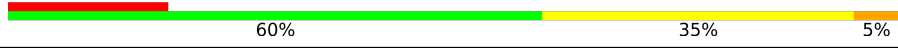
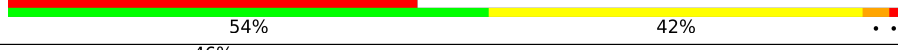
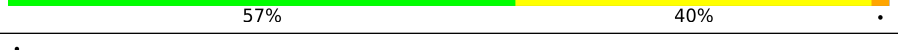
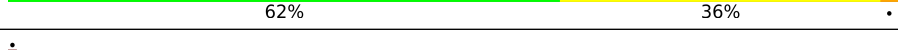
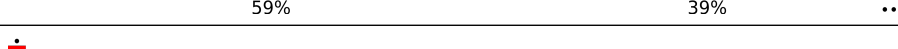
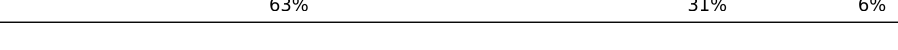
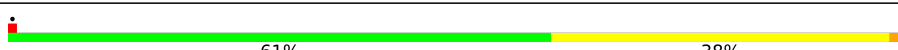
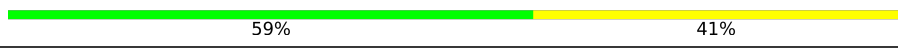
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 4585 ( 3.80 - 4.80 )                                     |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | b     | 271    |                  |
| 2   | c     | 209    |                  |
| 3   | d     | 201    |                  |

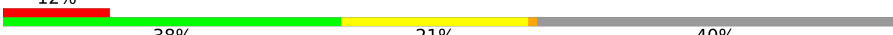
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | e     | 177    |    |
| 5   | f     | 176    |    |
| 6   | g     | 149    |    |
| 7   | h     | 131    |    |
| 8   | i     | 141    |    |
| 9   | j     | 142    |    |
| 10  | k     | 122    |    |
| 11  | l     | 143    |    |
| 12  | m     | 136    |    |
| 13  | n     | 120    |    |
| 14  | o     | 116    |    |
| 15  | p     | 114    |  |
| 16  | q     | 117    |  |
| 17  | r     | 103    |  |
| 18  | s     | 110    |  |
| 19  | t     | 93     |  |
| 20  | u     | 102    |  |
| 21  | v     | 94     |  |
| 22  | w     | 75     |  |
| 23  | x     | 77     |  |
| 24  | y     | 63     |  |
| 25  | z     | 58     |  |
| 26  | B     | 56     |  |
| 27  | C     | 50     |  |
| 28  | D     | 46     |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | E     | 64     |    |
| 30  | F     | 38     |    |
| 31  | G     | 225    |    |
| 32  | H     | 206    |    |
| 33  | I     | 205    |    |
| 34  | J     | 157    |    |
| 35  | K     | 100    |    |
| 36  | L     | 151    |    |
| 37  | M     | 129    |    |
| 38  | N     | 127    |    |
| 39  | O     | 98     |    |
| 40  | P     | 116    |   |
| 41  | Q     | 123    |  |
| 42  | R     | 114    |  |
| 43  | S     | 100    |  |
| 44  | T     | 88     |  |
| 45  | U     | 82     |  |
| 46  | V     | 80     |  |
| 47  | W     | 65     |  |
| 48  | X     | 79     |  |
| 49  | Y     | 85     |  |
| 50  | Z     | 65     |  |
| 51  | a     | 223    |  |
| 52  | 3     | 1539   |  |
| 53  | 1     | 2903   |  |

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| Mol | Chain | Length | Quality of chain                                                                      |
|-----|-------|--------|---------------------------------------------------------------------------------------|
| 54  | 2     | 120    | <div><div></div><div>57%</div><div>38%</div><div>6%</div></div>                       |
| 55  | 5     | 77     | <div><div>5%</div><div></div><div>78%</div><div>19%</div><div></div></div>            |
| 55  | 6     | 77     | <div><div>6%</div><div></div><div>64%</div><div>35%</div><div></div></div>            |
| 56  | 4     | 18     | <div><div>11%</div><div></div><div>61%</div><div>33%</div><div>6%</div></div>         |
| 57  | 7     | 76     | <div><div></div><div>76%</div><div></div><div>22%</div><div>7%</div><div></div></div> |

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 150149 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | g     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | h     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 989   | 625 | 175 | 184 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | i     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |       |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | B     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 27  | C     | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 410   | 263 | 75 | 72 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | D     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 29  | E     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30  | F     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 31 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 31  | G     | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1757  | 1111 | 315 | 323 | 8 |         |       |

- Molecule 32 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 32  | H     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1625  | 1028 | 305 | 289 | 3 |         |       |

- Molecule 33 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 33  | I     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 34 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | J     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1157  | 719 | 218 | 214 | 6 |         |       |

- Molecule 35 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | K     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 818   | 515 | 148 | 149 | 6 |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | L     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1182  | 735 | 227 | 216 | 4 |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | M     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 38 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | N     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 39 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | O     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 787   | 493 | 150 | 143 | 1 |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | P     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 870   | 535 | 173 | 159 | 3 |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | Q     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | R     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 884   | 546 | 178 | 157 | 3 |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | S     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | T     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 45 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | U     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 46 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | V     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 411 | 121 | 114 | 3 |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 47  | W     | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 536   | 339 | 100 | 96 | 1 |         |       |

- Molecule 48 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | X     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 638   | 408 | 120 | 108 | 2 |         |       |

- Molecule 49 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | Y     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |       |

- Molecule 50 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 50  | Z     | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 545   | 335 | 117 | 92 | 1 |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | a     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1027  | 645 | 186 | 194 | 2 |         |       |

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 52  | 3     | 1539     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33012 | 14725 | 6052 | 10697 | 1538 |         |       |

- Molecule 53 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 53  | 1     | 2903     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62317 | 27801 | 11468 | 20146 | 2902 |         |       |

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 54 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 54  | 2     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2568  | 1145 | 471 | 833 | 119 |         |       |

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 55 is a RNA chain called tRNA<sup>f</sup>Met.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 55  | 5     | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |       |
| 55  | 6     | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |       |

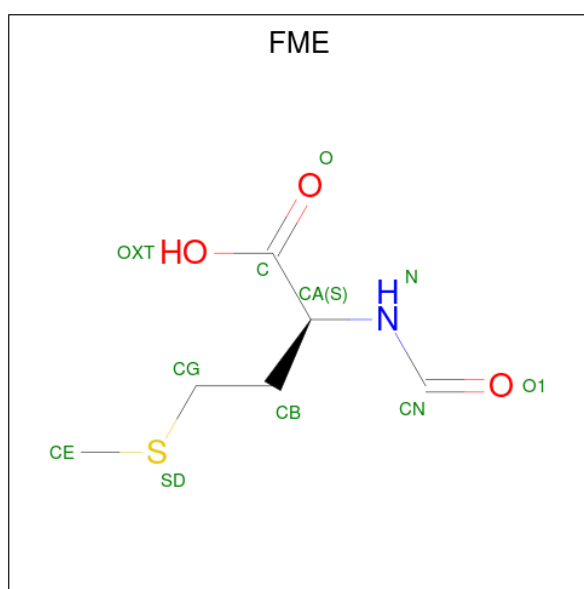
- Molecule 56 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 56  | 4     | 18       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 388   | 175 | 77 | 119 | 17 |         |       |

- Molecule 57 is a RNA chain called tRNA<sup>Phe</sup>.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 57  | 7     | 73       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1557  | 695 | 279 | 511 | 72 |         |       |

- Molecule 58 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).

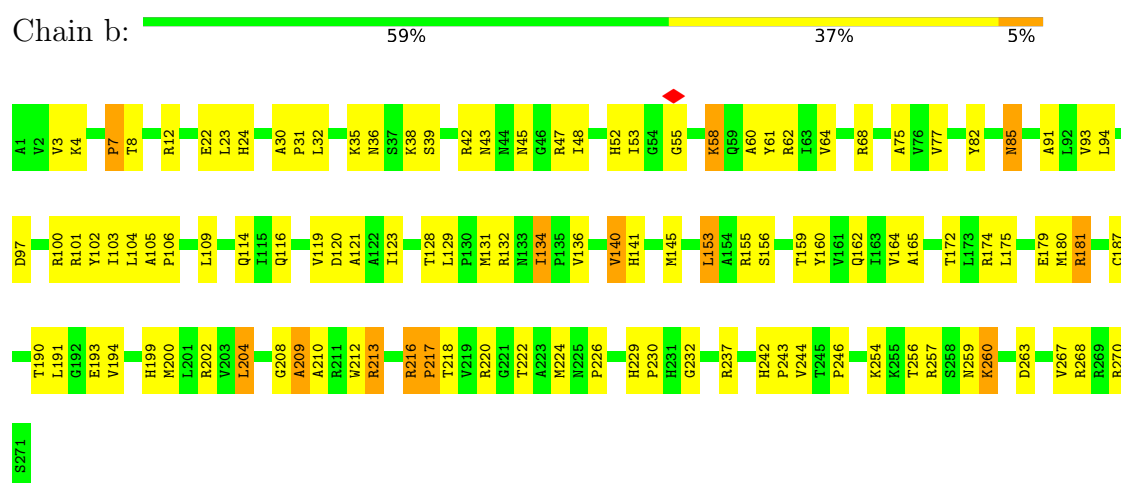


| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 58  | 5     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 10    | 6 | 1 | 2 | 1 |         |

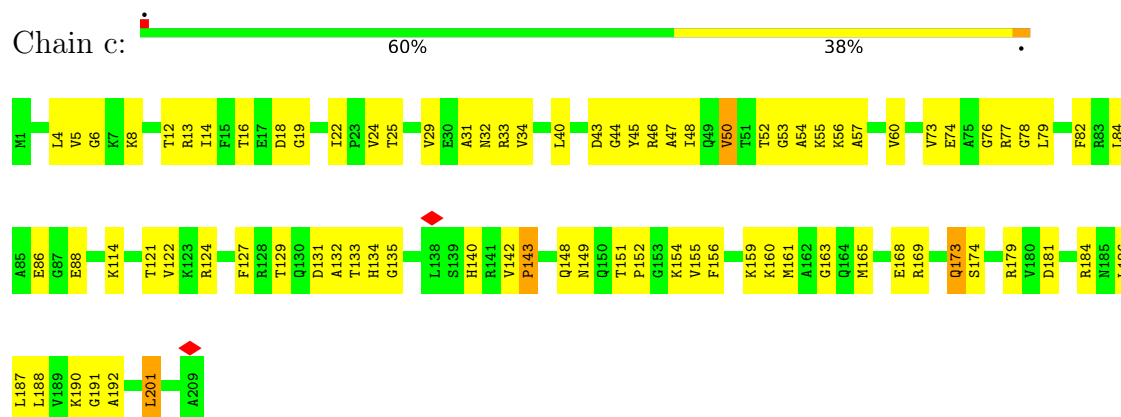
### 3 Residue-property plots

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

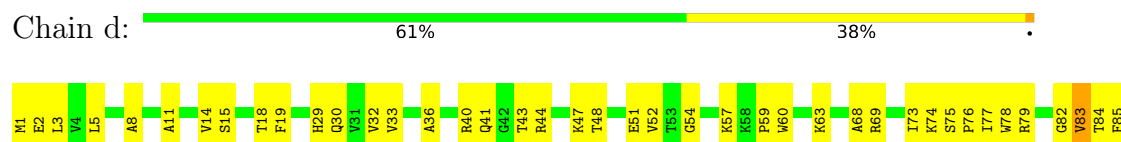
#### • Molecule 1: 50S ribosomal protein L2

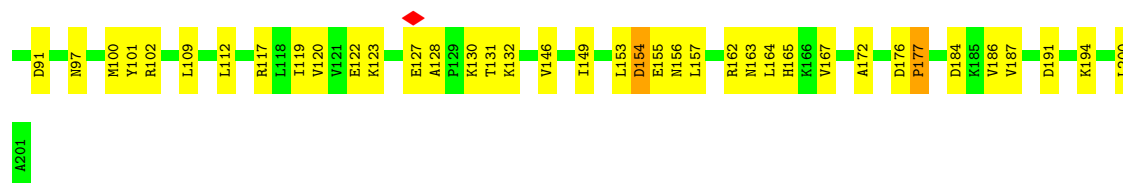


#### • Molecule 2: 50S ribosomal protein L3

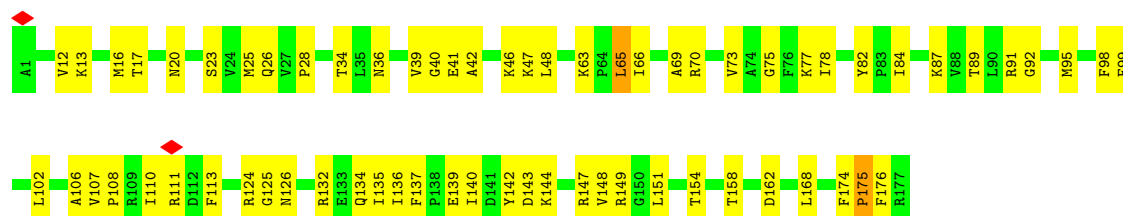


#### • Molecule 3: 50S ribosomal protein L4

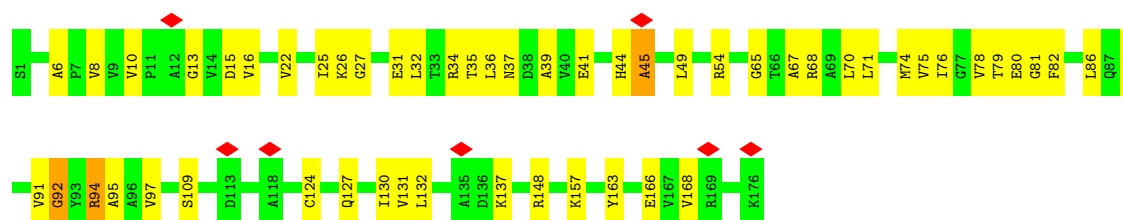




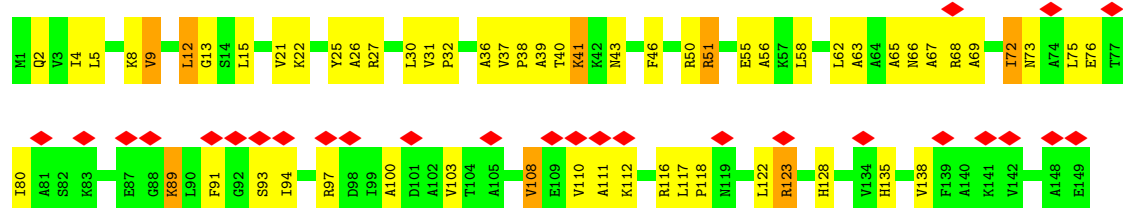
• Molecule 4: 50S ribosomal protein L5



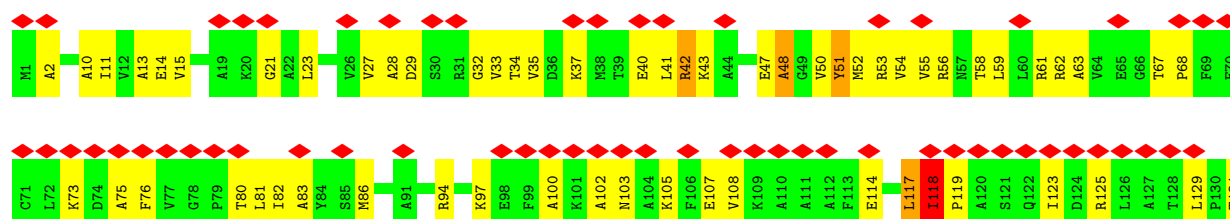
• Molecule 5: 50S ribosomal protein L6



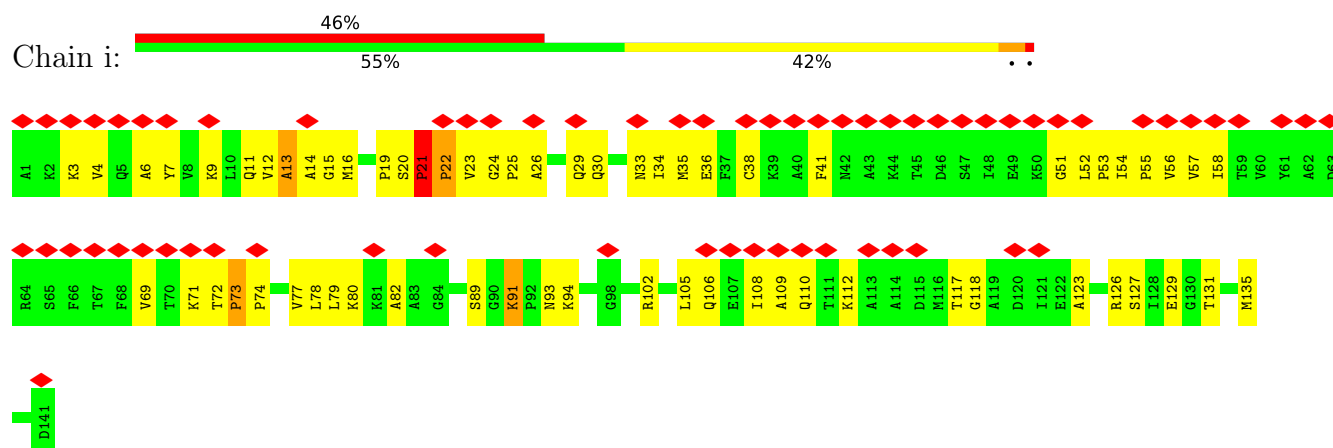
• Molecule 6: 50S ribosomal protein L9



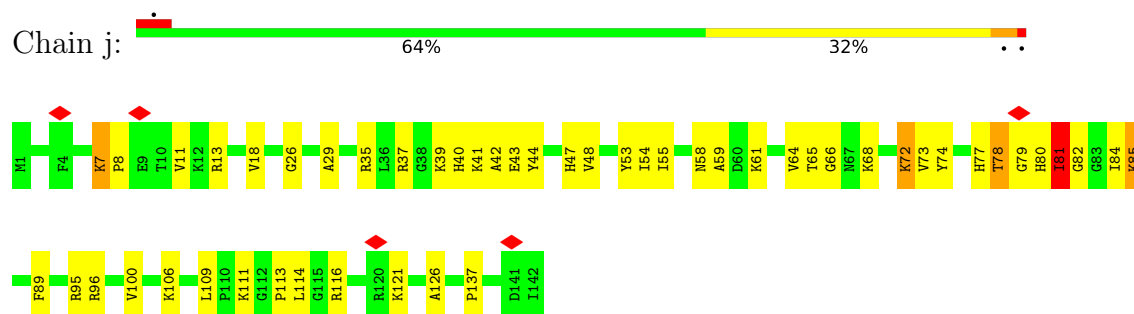
• Molecule 7: 50S ribosomal protein L10



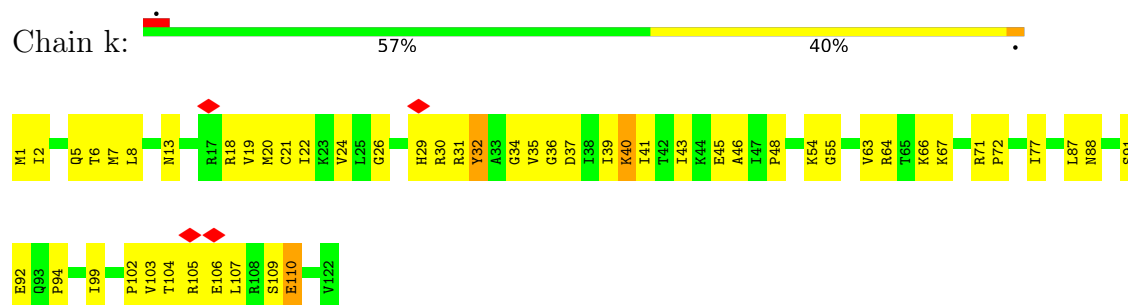
- Molecule 8: 50S ribosomal protein L11



- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14

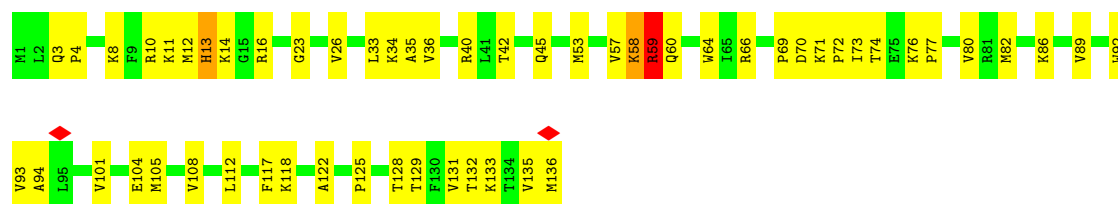


- Molecule 11: 50S ribosomal protein L15



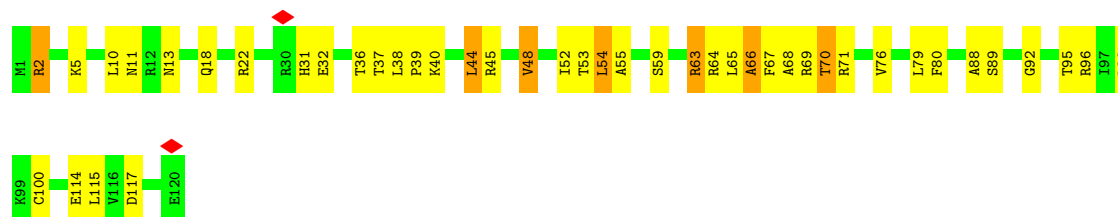
- Molecule 12: 50S ribosomal protein L16

Chain m: 



- Molecule 13: 50S ribosomal protein L17

Chain n: 



- Molecule 14: 50S ribosomal protein L18

Chain o: 



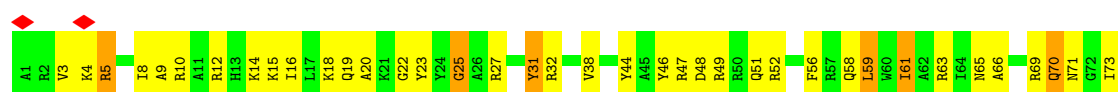
- Molecule 15: 50S ribosomal protein L19

Chain p: 



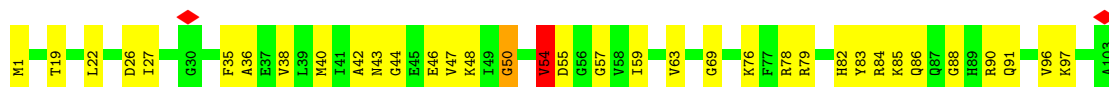
- Molecule 16: 50S ribosomal protein L20

Chain q: 





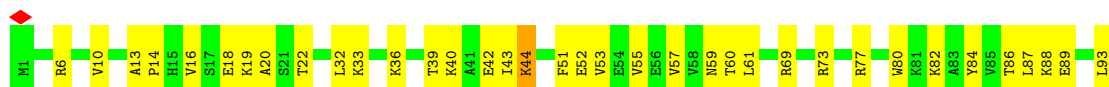
- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

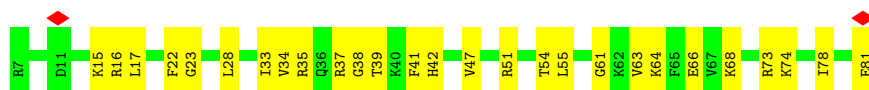


- Molecule 21: 50S ribosomal protein L25

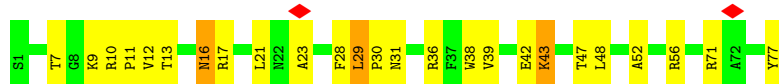


- Molecule 22: 50S ribosomal protein L27

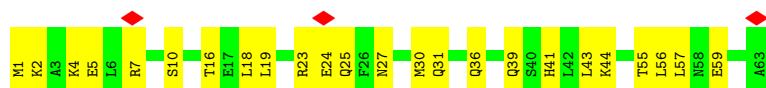




- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L34



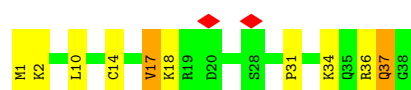
- Molecule 29: 50S ribosomal protein L35

Chain E: 



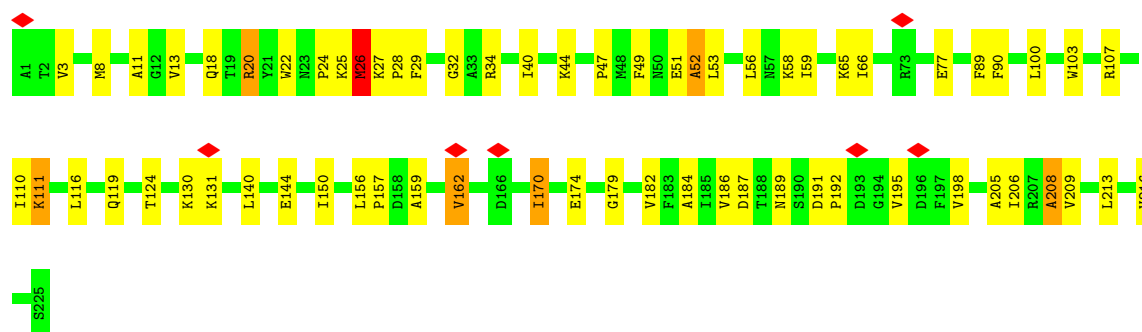
- Molecule 30: 50S ribosomal protein L36

Chain F: 



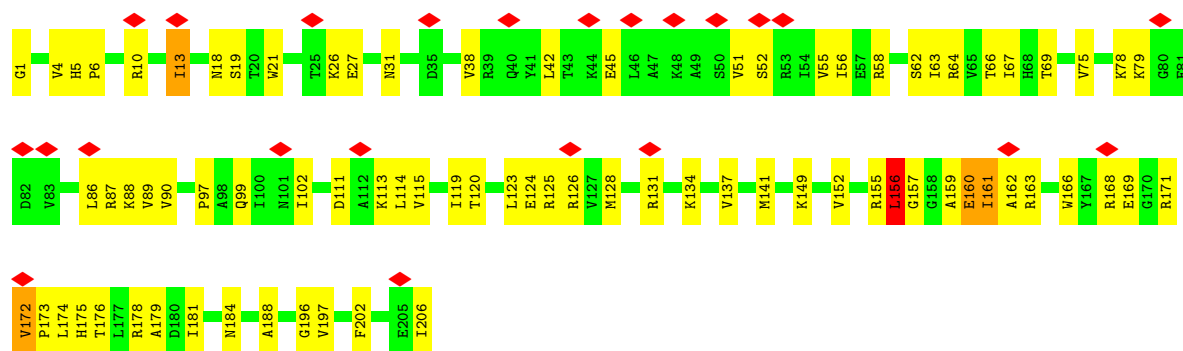
- Molecule 31: 30S ribosomal protein S2

Chain G: 



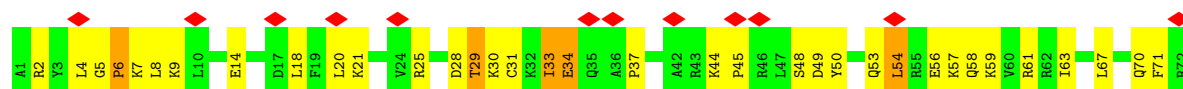
- Molecule 32: 30S ribosomal protein S3

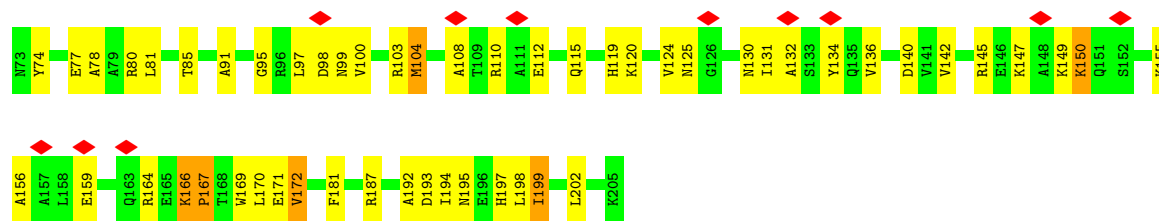
Chain H: 



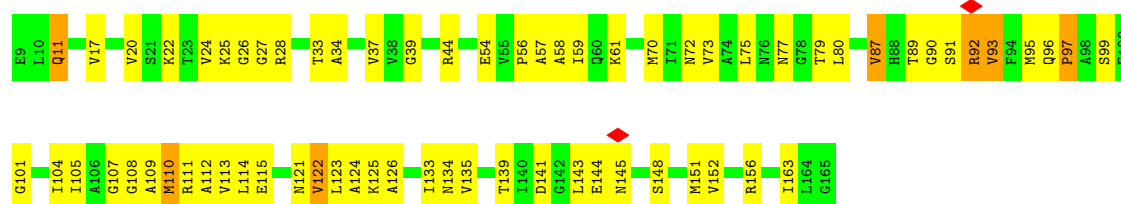
- Molecule 33: 30S ribosomal protein S4

Chain I: 

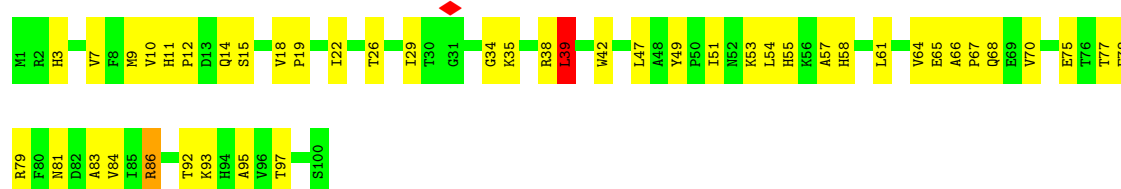




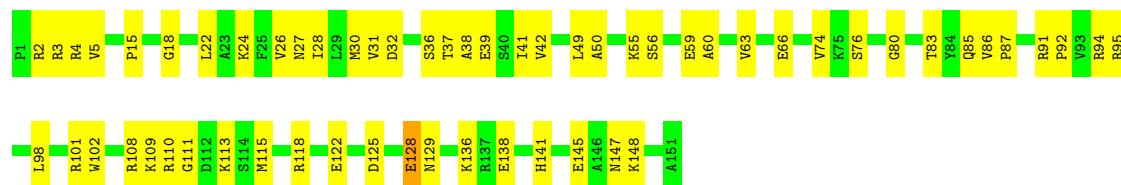
- Molecule 34: 30S ribosomal protein S5



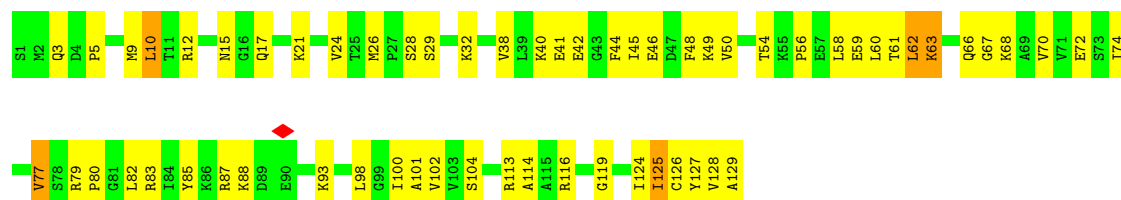
- Molecule 35: 30S ribosomal protein S6



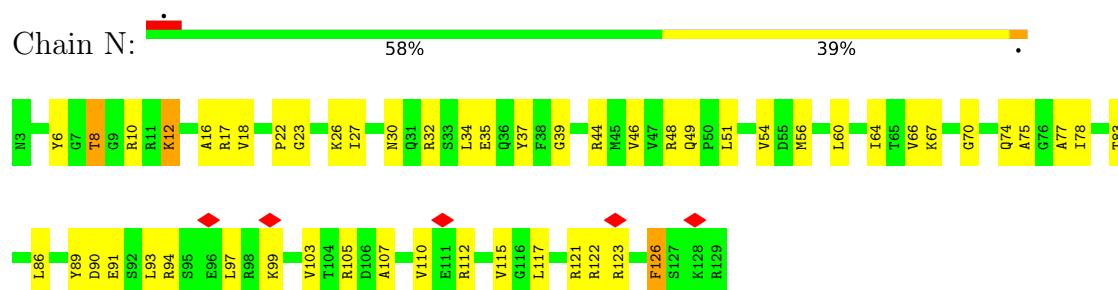
- Molecule 36: 30S ribosomal protein S7



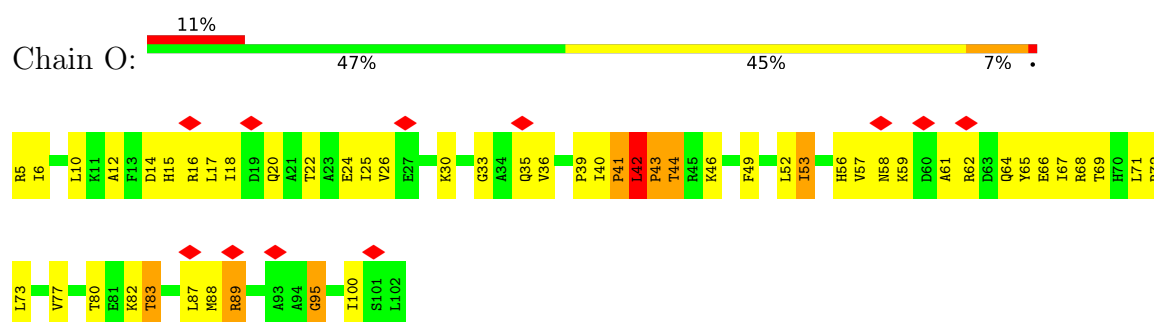
- Molecule 37: 30S ribosomal protein S8



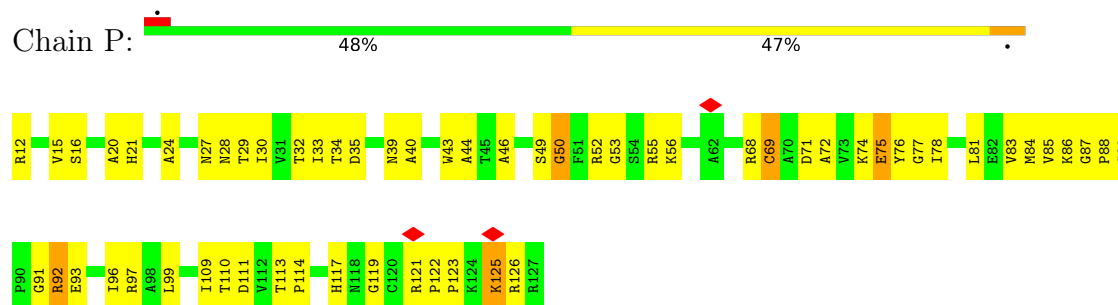
- Molecule 38: 30S ribosomal protein S9



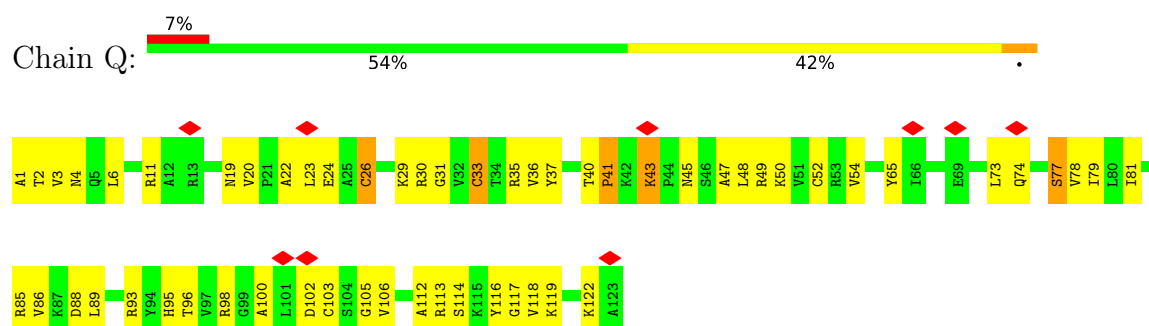
- Molecule 39: 30S ribosomal protein S10



- Molecule 40: 30S ribosomal protein S11

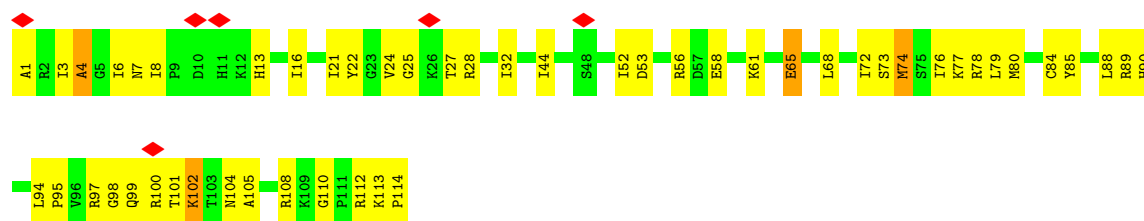


- Molecule 41: 30S ribosomal protein S12

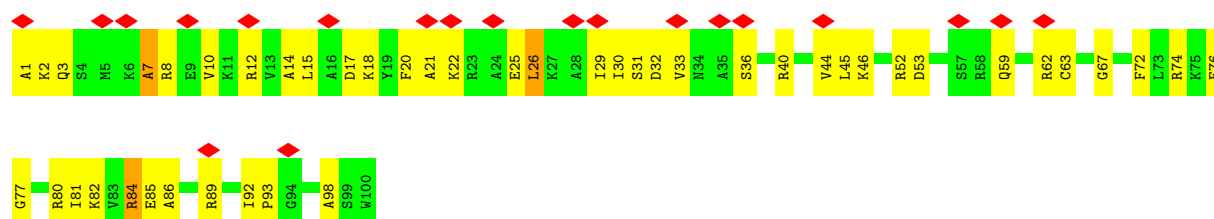


- Molecule 42: 30S ribosomal protein S13

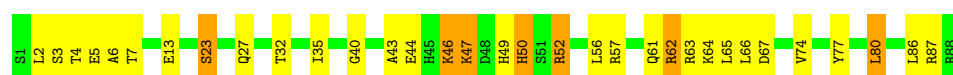




- Molecule 43: 30S ribosomal protein S14



- Molecule 44: 30S ribosomal protein S15



- Molecule 45: 30S ribosomal protein S16



- Molecule 46: 30S ribosomal protein S17

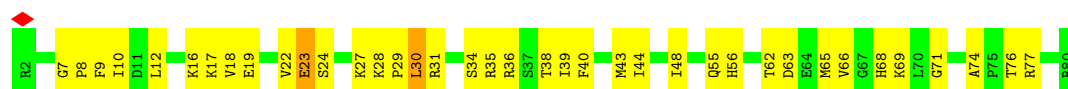


- Molecule 47: 30S ribosomal protein S18



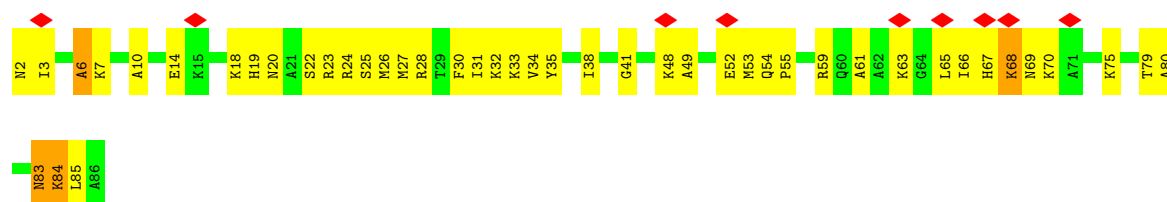
- Molecule 48: 30S ribosomal protein S19

Chain X: 



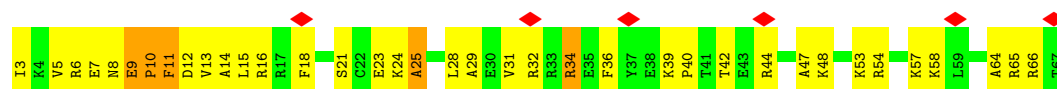
- Molecule 49: 30S ribosomal protein S20

Chain Y: 

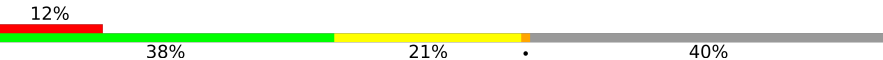


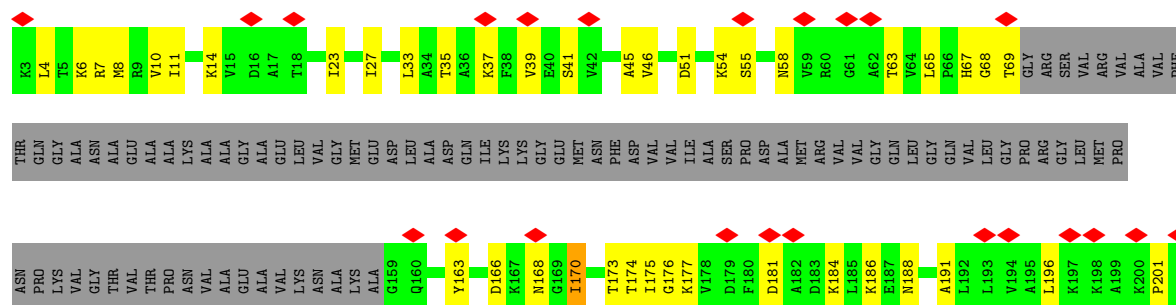
- Molecule 50: 30S ribosomal protein S21

Chain Z: 



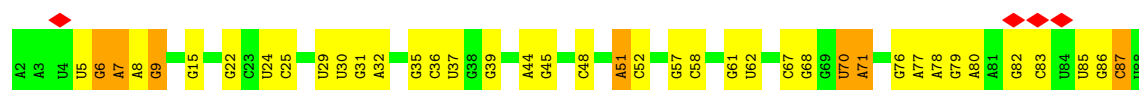
- Molecule 51: 50S ribosomal protein L1

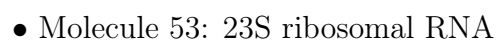
Chain a: 



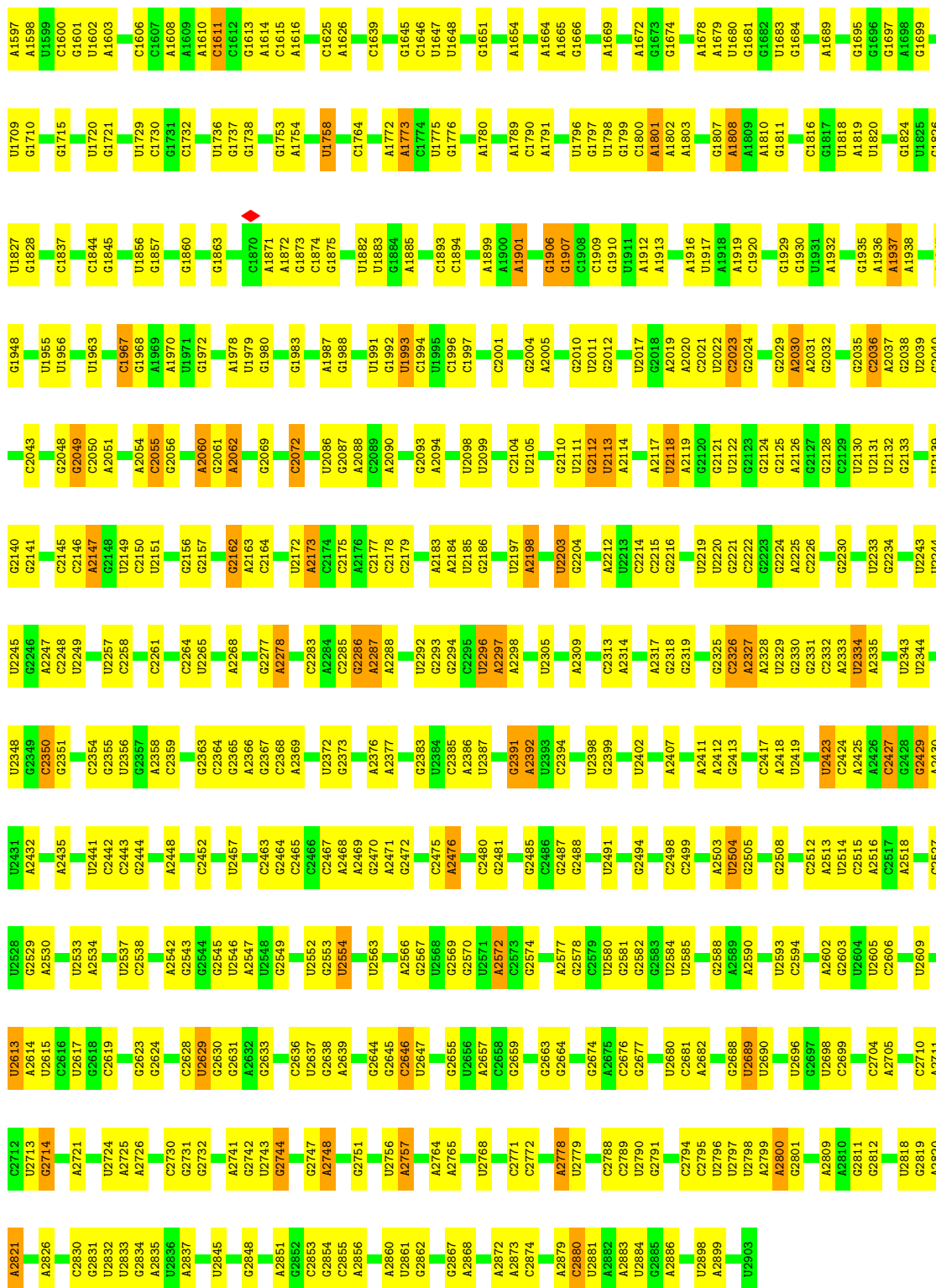
- Molecule 52: 16S ribosomal RNA

Chain 3: 





|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|
| C1498 | C1499 | G1500 | A1509 | C1510 | G1511 | A1515 | G1524 | A1525 | C1526 | G1527 | A1528 | G1529 | A1535 | C1536 | G1537 | C1538 | A1539 | C1540 | C1541 | U1542 | G1543 | C1547 | A1548 | A1551 | A1552 | A1553 | U1554 | G1555 | C1558 | U1559 | G1560 | C1561 | U1562 | A1566 | G1567 | A1569 | A1570 | A1571 | A1580 | G1581 | U1584 | C1585 | A1586 | G1587 | A1590 | C1591 |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| G1368 | G1369 | C1370 | G1371 | G1372 | A1373 | C1376 | G1377 | A1378 | U1379 | G1380 | A1383 | C1398 | U1415 | C1416 | C1417 | G1418 | U1419 | A1420 | G1424 | G1425 | G1429 | A1430 | A1431 | G1432 | A1433 | A1434 | G1435 | U1440 | G1441 | U1442 | U1443 | G1444 | G1445 | C1454 | C1461 | U1474 | G1475 | U1476 | G1482 | U1487 | C1488 | A1489 | A1490 | G1491 | G1492 | A1493 |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| A1264 | A1268 | A1269 | G1270 | G1271 | A1272 | A1275 | C1278 | G1279 | C1289 | G1296 | C1297 | C1298 | G1299 | G1300 | A1301 | A1302 | C1306 | G1309 | U1313 | C1319 | C1320 | A1321 | A1322 | C1323 | U1329 | C1330 | G1331 | G1332 | G1333 | C1334 | C1335 | G1339 | U1340 | G1341 | U1344 | C1345 | G1355 | G1356 | C1357 | G1358 | A1359 | G1360 | A1365 | A1366 | A1367 |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| G1157 | G1162 | G1163 | C1170 | G1171 | A1175 | U1176 | G1177 | C1178 | A1077 | U1078 | A1080 | U1081 | U1082 | U1083 | G1186 | G1187 | U1188 | A1189 | G1190 | U1201 | G1202 | G1430 | A1431 | G1432 | A1433 | A1434 | G1435 | U1440 | G1441 | U1442 | U1443 | G1444 | G1445 | G1225 | U1231 | G1232 | C1233 | U1234 | G1235 | G1248 | C1251 | G1252 | A1253 | A1254 | U1255 | G1256 | C1257 | U1258 | G1259 |      |      |      |      |      |      |      |      |      |      |      |      |
| U1058 | G1059 | U1060 | U1061 | G1062 | U1066 | A1067 | A1070 | G1071 | A1077 | U1078 | A1080 | U1081 | U1082 | U1083 | A1086 | A1087 | C888  | G891  | A896  | C897  | A905  | U906  | A909  | A910  | C911  | U912  | U913  | A917  | C922  | U932  | C937  | G938  | G939  | G940  | A941  | G942  | A943  | C946  | A947  | C948  | G949  | G953  | C954  | U955  |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| G956  | C957  | C961  | G962  | U967  | C968  | G969  | G974  | A975  | A983  | A990  | C991  | C992  | C995  | A996  | C997  | A1001 | G1002 | A1009 | U1012 | C1013 | A1014 | U1019 | A1020 | A1021 | C1022 | U1023 | G1026 | A1027 | U1033 | G1034 | U1035 | G1036 | A1040 | C1043 | C1044 | C1045 | A1046 | G1047 | C1052 | C1053 | A1054 | G1055 | G1056 | A1057 |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| U058  | G059  | U060  | A061  | G062  | A068  | G069  | A070  | C080  | G081  | G082  | A085  | U086  | C087  | U088  | A089  | C090  | C091  | C092  | G095  | A099  | G000  | U003  | G004  | G005  | G006  | U007  | A015  | A018  | C019  | U020  | A021  | C022  | G023  | A024  | G027  | G028  | A029  | G030  | C031  | A032  | G033  | C034  | G035  | G036  | U037  | A041  | A042  | A043  | A044  | C045 | C046 | U047 | A048 | A049 | A050 | A051 | A052 | A053 | A054 | A055 | A056 |
| C239  | C240  | A241  | A244  | G248  | C249  | G250  | A251  | G252  | C253  | G254  | A255  | A256  | A265  | G266  | C274  | C275  | U276  | G277  | A278  | C281  | U293  | A294  | G297  | G301  | G307  | A310  | A311  | G319  | A320  | U321  | A322  | C323  | A324  | G325  | G326  | G327  | U328  | A330  | C331  | C336  | G337  | G338  | U339  | A340  | C341  | A342  |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
| C343  | A344  | A345  | A346  | A362  | G363  | G367  | A368  | A371  | G372  | A382  | A483  | C484  | G488  | C489  | C490  | C491  | A492  | G493  | G494  | U499  | A503  | A504  | A505  | G506  | C509  | C510  | U511  | G512  | G518  | U519  | G520  | A529  | G530  | C531  | A532  | G533  | C534  | G535  | C542  | G543  | C544  | U545  | U546  | A547  | G548  | G549  | U554  | G555  | A556  |      |      |      |      |      |      |      |      |      |      |      |      |
| C433  | A434  | A435  | A436  | A462  | G463  | G467  | A468  | A477  | A478  | A479  | A480  | C481  | A482  | A483  | C484  | G488  | C489  | C490  | C491  | A492  | G493  | G494  | U499  | A503  | A504  | A505  | G506  | C509  | C510  | U511  | G512  | G518  | U519  | G520  | A529  | G530  | C531  | A532  | G533  | C534  | G535  | C542  | G543  | C544  | U545  | U546  | A547  | G548  | G549  | U554 | G555 | A556 |      |      |      |      |      |      |      |      |      |
| C433  | A434  | A435  | A436  | A462  | G463  | G467  | A468  | A477  | A478  | A479  | A480  | C481  | A482  | A483  | C484  | G488  | C489  | C490  | C491  | A492  | G493  | G494  | U499  | A503  | A504  | A505  | G506  | C509  | C510  | U511  | G512  | G518  | U519  | G520  | A529  | G530  | C531  | A532  | G533  | C534  | G535  | C542  | G543  | C544  | U545  | U546  | A547  | G548  | G549  | U554 | G555 | A556 |      |      |      |      |      |      |      |      |      |



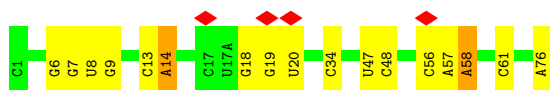
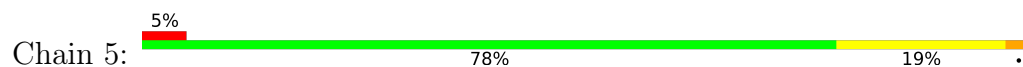
• Molecule 54: 5S ribosomal RNA

Chain 2: 57% 38% 6%

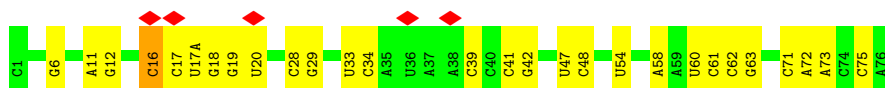




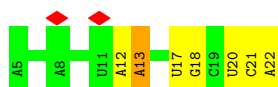
## • Molecule 55: tRNAfMet



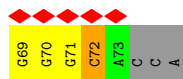
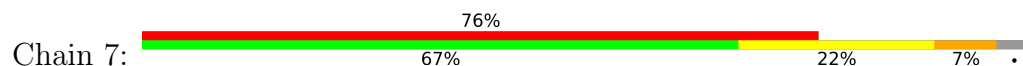
## • Molecule 55: tRNAfMet



## • Molecule 56: mRNA



## • Molecule 57: tRNAPhe



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 1699                                    | 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 ( $e^-/\text{\AA}^2$ ) | 35                                      | 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                    | 18.877                                  | Depositor |
| Minimum map value                    | -10.681                                 | Depositor |
| Average map value                    | 0.115                                   | Depositor |
| Map value standard deviation         | 0.882                                   | Depositor |
| Recommended contour level            | 1                                       | Depositor |
| Map size (Å)                         | 383.904, 383.904, 383.904               | wwPDB     |
| Map dimensions                       | 288, 288, 288                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.333, 1.333, 1.333                     | Depositor |

## 5 Model quality [i](#)

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

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$    |
| 1   | b     | 0.30         | 0/2122      | 0.98        | 11/2852 (0.4%) |
| 2   | c     | 0.30         | 0/1586      | 0.85        | 2/2134 (0.1%)  |
| 3   | d     | 0.30         | 0/1571      | 0.94        | 5/2113 (0.2%)  |
| 4   | e     | 0.31         | 0/1435      | 0.91        | 4/1926 (0.2%)  |
| 5   | f     | 0.30         | 0/1343      | 0.95        | 9/1816 (0.5%)  |
| 6   | g     | 0.30         | 0/1122      | 1.01        | 8/1515 (0.5%)  |
| 7   | h     | 0.33         | 0/1002      | 1.02        | 3/1350 (0.2%)  |
| 8   | i     | 0.37         | 0/1046      | 1.01        | 10/1410 (0.7%) |
| 9   | j     | 0.30         | 0/1152      | 0.95        | 7/1551 (0.5%)  |
| 10  | k     | 0.30         | 0/948       | 1.00        | 3/1268 (0.2%)  |
| 11  | l     | 0.30         | 0/1054      | 1.00        | 5/1403 (0.4%)  |
| 12  | m     | 0.32         | 0/1093      | 0.95        | 3/1460 (0.2%)  |
| 13  | n     | 0.32         | 0/974       | 1.02        | 10/1301 (0.8%) |
| 14  | o     | 0.29         | 0/902       | 0.95        | 3/1209 (0.2%)  |
| 15  | p     | 0.30         | 0/929       | 0.88        | 3/1242 (0.2%)  |
| 16  | q     | 0.29         | 0/960       | 0.96        | 8/1278 (0.6%)  |
| 17  | r     | 0.30         | 0/829       | 0.99        | 4/1107 (0.4%)  |
| 18  | s     | 0.27         | 0/864       | 0.94        | 1/1156 (0.1%)  |
| 19  | t     | 0.29         | 0/745       | 1.02        | 4/994 (0.4%)   |
| 20  | u     | 0.31         | 0/788       | 1.01        | 5/1051 (0.5%)  |
| 21  | v     | 0.29         | 0/766       | 0.89        | 3/1025 (0.3%)  |
| 22  | w     | 0.31         | 0/582       | 0.90        | 1/769 (0.1%)   |
| 23  | x     | 0.30         | 0/635       | 0.89        | 0/848          |
| 24  | y     | 0.29         | 0/510       | 1.06        | 6/677 (0.9%)   |
| 25  | z     | 0.30         | 0/453       | 1.06        | 4/605 (0.7%)   |
| 26  | B     | 0.28         | 0/450       | 0.82        | 2/599 (0.3%)   |
| 27  | C     | 0.34         | 0/417       | 0.82        | 0/554          |
| 28  | D     | 0.32         | 0/380       | 0.92        | 1/498 (0.2%)   |
| 29  | E     | 0.30         | 0/513       | 0.91        | 1/676 (0.1%)   |
| 30  | F     | 0.31         | 0/303       | 0.92        | 0/397          |
| 31  | G     | 0.29         | 0/1788      | 0.96        | 10/2408 (0.4%) |
| 32  | H     | 0.30         | 0/1652      | 0.97        | 8/2225 (0.4%)  |

| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 33  | I     | 0.29         | 0/1665   | 1.02        | 11/2227 (0.5%)    |
| 34  | J     | 0.34         | 0/1170   | 0.97        | 6/1573 (0.4%)     |
| 35  | K     | 0.30         | 0/836    | 0.97        | 3/1128 (0.3%)     |
| 36  | L     | 0.29         | 0/1196   | 0.90        | 1/1602 (0.1%)     |
| 37  | M     | 0.30         | 0/989    | 0.90        | 3/1326 (0.2%)     |
| 38  | N     | 0.30         | 0/1034   | 0.93        | 2/1375 (0.1%)     |
| 39  | O     | 0.32         | 0/797    | 0.99        | 7/1077 (0.6%)     |
| 40  | P     | 0.31         | 0/886    | 0.99        | 5/1195 (0.4%)     |
| 41  | Q     | 0.30         | 0/969    | 1.02        | 6/1300 (0.5%)     |
| 42  | R     | 0.32         | 0/893    | 0.99        | 5/1193 (0.4%)     |
| 43  | S     | 0.29         | 0/817    | 0.96        | 4/1088 (0.4%)     |
| 44  | T     | 0.29         | 0/722    | 0.99        | 5/964 (0.5%)      |
| 45  | U     | 0.33         | 0/659    | 1.03        | 3/884 (0.3%)      |
| 46  | V     | 0.29         | 0/658    | 0.89        | 2/881 (0.2%)      |
| 47  | W     | 0.32         | 0/545    | 0.92        | 1/731 (0.1%)      |
| 48  | X     | 0.31         | 0/653    | 0.90        | 2/877 (0.2%)      |
| 49  | Y     | 0.29         | 0/671    | 1.06        | 7/888 (0.8%)      |
| 50  | Z     | 0.34         | 0/551    | 1.03        | 4/728 (0.5%)      |
| 51  | a     | 0.32         | 0/1034   | 0.85        | 1/1387 (0.1%)     |
| 52  | 3     | 0.40         | 0/36963  | 0.51        | 3/57662 (0.0%)    |
| 53  | 1     | 0.39         | 0/69796  | 0.50        | 1/108888 (0.0%)   |
| 54  | 2     | 0.40         | 0/2872   | 0.51        | 0/4479            |
| 55  | 5     | 0.39         | 0/1832   | 0.49        | 0/2855            |
| 55  | 6     | 0.39         | 0/1832   | 0.51        | 0/2855            |
| 56  | 4     | 0.40         | 0/436    | 0.48        | 0/679             |
| 57  | 7     | 0.40         | 0/1740   | 0.50        | 0/2712            |
| All | All   | 0.37         | 0/163130 | 0.65        | 226/243971 (0.1%) |

There are no bond length outliers.

All (226) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 17  | r     | 50  | GLY  | N-CA-C | -9.72 | 102.40      | 114.16   |
| 31  | G     | 20  | ARG  | N-CA-C | -8.80 | 102.67      | 113.50   |
| 34  | J     | 92  | ARG  | N-CA-C | -8.70 | 102.80      | 113.50   |
| 6   | g     | 72  | ILE  | N-CA-C | -8.33 | 102.75      | 111.58   |
| 7   | h     | 117 | LEU  | N-CA-C | 8.27  | 123.12      | 109.06   |
| 9   | j     | 79  | GLY  | N-CA-C | -8.12 | 103.30      | 115.00   |
| 40  | P     | 75  | GLU  | N-CA-C | -8.12 | 102.40      | 111.82   |
| 18  | s     | 42  | LYS  | N-CA-C | -7.91 | 102.26      | 112.23   |
| 1   | b     | 12  | ARG  | N-CA-C | -7.88 | 103.38      | 113.16   |
| 9   | j     | 78  | THR  | N-CA-C | 7.82  | 119.80      | 111.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 16  | q     | 16  | ILE  | N-CA-C | -7.73 | 105.16      | 111.81   |
| 12  | m     | 135 | VAL  | N-CA-C | 7.69  | 114.44      | 106.21   |
| 11  | l     | 95  | LEU  | N-CA-C | -7.49 | 102.80      | 112.23   |
| 20  | u     | 76  | THR  | N-CA-C | -7.41 | 104.27      | 113.38   |
| 41  | Q     | 26  | CYS  | CA-C-N | 7.38  | 127.73      | 119.32   |
| 41  | Q     | 26  | CYS  | C-N-CA | 7.38  | 127.73      | 119.32   |
| 21  | v     | 80  | HIS  | N-CA-C | -7.37 | 100.51      | 109.72   |
| 44  | T     | 50  | HIS  | N-CA-C | -7.26 | 103.39      | 112.90   |
| 13  | n     | 88  | ALA  | N-CA-C | 7.22  | 118.80      | 111.07   |
| 40  | P     | 69  | CYS  | N-CA-C | -7.22 | 104.73      | 113.97   |
| 2   | c     | 173 | GLN  | N-CA-C | 7.18  | 121.73      | 110.32   |
| 49  | Y     | 3   | ILE  | N-CA-C | 7.07  | 113.77      | 106.21   |
| 41  | Q     | 114 | SER  | N-CA-C | -7.06 | 103.67      | 111.36   |
| 45  | U     | 62  | GLY  | N-CA-C | -7.02 | 105.95      | 114.66   |
| 32  | H     | 160 | GLU  | N-CA-C | 7.01  | 118.81      | 111.03   |
| 3   | d     | 146 | VAL  | N-CA-C | 7.00  | 119.23      | 109.29   |
| 7   | h     | 42  | ARG  | N-CA-C | -7.00 | 104.21      | 112.89   |
| 31  | G     | 77  | GLU  | N-CA-C | 6.97  | 118.96      | 111.36   |
| 13  | n     | 63  | ARG  | N-CA-C | -6.91 | 103.81      | 111.82   |
| 20  | u     | 75  | ALA  | N-CA-C | -6.89 | 103.77      | 112.93   |
| 11  | l     | 96  | LYS  | N-CA-C | -6.88 | 103.84      | 111.82   |
| 43  | S     | 22  | LYS  | N-CA-C | -6.85 | 105.48      | 114.31   |
| 35  | K     | 39  | LEU  | N-CA-C | -6.80 | 102.05      | 112.99   |
| 49  | Y     | 69  | ASN  | N-CA-C | -6.79 | 103.68      | 112.23   |
| 24  | y     | 44  | LYS  | N-CA-C | 6.76  | 118.34      | 110.97   |
| 14  | o     | 20  | GLU  | N-CA-C | -6.71 | 105.22      | 113.41   |
| 11  | l     | 92  | LEU  | N-CA-C | -6.67 | 104.40      | 112.54   |
| 40  | P     | 50  | GLY  | N-CA-C | -6.67 | 101.31      | 111.24   |
| 11  | l     | 43  | GLY  | N-CA-C | -6.61 | 106.11      | 115.43   |
| 25  | z     | 52  | PHE  | N-CA-C | 6.59  | 119.28      | 111.71   |
| 6   | g     | 123 | ARG  | N-CA-C | -6.54 | 105.59      | 113.97   |
| 5   | f     | 45  | ALA  | N-CA-C | -6.54 | 103.79      | 113.40   |
| 19  | t     | 19  | LYS  | N-CA-C | -6.53 | 104.89      | 112.92   |
| 50  | Z     | 54  | ARG  | N-CA-C | -6.51 | 104.26      | 111.82   |
| 41  | Q     | 19  | ASN  | N-CA-C | -6.51 | 104.59      | 112.54   |
| 33  | I     | 104 | MET  | N-CA-C | -6.50 | 105.47      | 113.41   |
| 8   | i     | 127 | SER  | N-CA-C | -6.42 | 104.14      | 112.23   |
| 44  | T     | 43  | ALA  | N-CA-C | -6.36 | 104.21      | 112.23   |
| 25  | z     | 17  | PRO  | N-CA-C | -6.34 | 105.60      | 113.84   |
| 8   | i     | 91  | LYS  | CA-C-N | 6.33  | 125.82      | 119.24   |
| 8   | i     | 91  | LYS  | C-N-CA | 6.33  | 125.82      | 119.24   |
| 44  | T     | 40  | GLY  | N-CA-C | -6.31 | 104.91      | 113.37   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 19  | t     | 36  | LYS  | N-CA-C | 6.31  | 118.16      | 111.28   |
| 5   | f     | 13  | GLY  | N-CA-C | -6.26 | 107.24      | 114.69   |
| 38  | N     | 103 | VAL  | N-CA-C | -6.26 | 105.52      | 113.22   |
| 17  | r     | 54  | VAL  | N-CA-C | 6.24  | 122.32      | 109.34   |
| 3   | d     | 73  | ILE  | N-CA-C | -6.24 | 105.62      | 112.80   |
| 26  | B     | 46  | GLY  | N-CA-C | 6.24  | 124.23      | 115.43   |
| 16  | q     | 3   | VAL  | N-CA-C | 6.22  | 116.83      | 107.75   |
| 6   | g     | 51  | ARG  | N-CA-C | 6.20  | 118.04      | 111.28   |
| 13  | n     | 67  | PHE  | N-CA-C | -6.19 | 106.27      | 113.88   |
| 31  | G     | 162 | VAL  | N-CA-C | 6.17  | 117.48      | 108.53   |
| 50  | Z     | 42  | THR  | N-CA-C | 6.15  | 117.65      | 111.07   |
| 17  | r     | 36  | ALA  | N-CA-C | -6.14 | 104.96      | 112.88   |
| 8   | i     | 110 | GLN  | N-CA-C | -6.14 | 104.14      | 111.69   |
| 1   | b     | 134 | ILE  | N-CA-C | 6.12  | 114.95      | 108.95   |
| 4   | e     | 174 | PHE  | CA-C-N | 6.12  | 127.49      | 119.84   |
| 4   | e     | 174 | PHE  | C-N-CA | 6.12  | 127.49      | 119.84   |
| 49  | Y     | 18  | LYS  | N-CA-C | -6.10 | 104.55      | 111.14   |
| 1   | b     | 216 | ARG  | CA-C-N | 6.10  | 127.46      | 119.84   |
| 1   | b     | 216 | ARG  | C-N-CA | 6.10  | 127.46      | 119.84   |
| 41  | Q     | 43  | LYS  | N-CA-C | 6.08  | 123.24      | 109.81   |
| 33  | I     | 33  | ILE  | N-CA-C | 6.07  | 117.07      | 110.21   |
| 16  | q     | 71  | ASN  | N-CA-C | -6.07 | 105.88      | 113.28   |
| 47  | W     | 41  | SER  | N-CA-C | 6.04  | 117.53      | 111.07   |
| 48  | X     | 30  | LEU  | N-CA-C | 6.02  | 119.09      | 110.24   |
| 37  | M     | 15  | ASN  | N-CA-C | -5.99 | 105.94      | 113.18   |
| 5   | f     | 109 | SER  | N-CA-C | -5.98 | 105.29      | 112.59   |
| 8   | i     | 21  | PRO  | N-CA-C | 5.98  | 117.99      | 110.70   |
| 39  | O     | 95  | GLY  | N-CA-C | -5.98 | 107.15      | 114.92   |
| 45  | U     | 78  | VAL  | N-CA-C | -5.95 | 105.58      | 111.77   |
| 33  | I     | 166 | LYS  | CA-C-N | 5.94  | 127.27      | 119.84   |
| 33  | I     | 166 | LYS  | C-N-CA | 5.94  | 127.27      | 119.84   |
| 1   | b     | 22  | GLU  | N-CA-C | -5.93 | 104.81      | 111.28   |
| 19  | t     | 13  | ALA  | N-CA-C | 5.93  | 113.47      | 108.13   |
| 28  | D     | 42  | LEU  | N-CA-C | -5.92 | 104.74      | 111.07   |
| 6   | g     | 27  | ARG  | N-CA-C | 5.91  | 117.80      | 111.36   |
| 34  | J     | 110 | MET  | N-CA-C | -5.91 | 104.97      | 111.82   |
| 42  | R     | 73  | SER  | N-CA-C | -5.90 | 104.97      | 111.82   |
| 34  | J     | 145 | ASN  | N-CA-C | -5.88 | 106.10      | 113.28   |
| 39  | O     | 53  | ILE  | N-CA-C | 5.88  | 117.15      | 111.91   |
| 43  | S     | 85  | GLU  | N-CA-C | -5.88 | 106.34      | 112.93   |
| 39  | O     | 77  | VAL  | N-CA-C | 5.87  | 116.05      | 110.53   |
| 9   | j     | 81  | ILE  | N-CA-C | 5.87  | 121.55      | 109.34   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 41  | Q     | 105 | GLY  | N-CA-C | -5.86 | 103.57      | 111.54   |
| 10  | k     | 32  | TYR  | N-CA-C | 5.86  | 118.27      | 108.96   |
| 51  | a     | 191 | ALA  | N-CA-C | -5.83 | 105.06      | 111.82   |
| 43  | S     | 84  | ARG  | N-CA-C | -5.81 | 104.91      | 112.23   |
| 8   | i     | 24  | GLY  | CA-C-N | 5.80  | 125.50      | 119.82   |
| 8   | i     | 24  | GLY  | C-N-CA | 5.80  | 125.50      | 119.82   |
| 16  | q     | 31  | TYR  | N-CA-C | 5.79  | 117.27      | 111.07   |
| 1   | b     | 213 | ARG  | N-CA-C | -5.78 | 104.42      | 112.45   |
| 50  | Z     | 11  | PHE  | N-CA-C | -5.74 | 105.94      | 113.12   |
| 15  | p     | 14  | GLN  | N-CA-C | 5.74  | 117.21      | 111.07   |
| 37  | M     | 114 | ALA  | N-CA-C | -5.73 | 105.40      | 112.90   |
| 13  | n     | 66  | ALA  | N-CA-C | -5.71 | 106.08      | 113.16   |
| 31  | G     | 52  | ALA  | N-CA-C | -5.70 | 104.68      | 111.69   |
| 9   | j     | 7   | LYS  | CA-C-N | 5.68  | 125.36      | 119.56   |
| 9   | j     | 7   | LYS  | C-N-CA | 5.68  | 125.36      | 119.56   |
| 35  | K     | 42  | TRP  | N-CA-C | -5.68 | 105.85      | 112.89   |
| 49  | Y     | 84  | LYS  | N-CA-C | -5.68 | 105.08      | 112.23   |
| 12  | m     | 59  | ARG  | N-CA-C | 5.65  | 122.83      | 110.80   |
| 14  | o     | 54  | VAL  | N-CA-C | -5.62 | 105.42      | 113.07   |
| 1   | b     | 134 | ILE  | CA-C-N | 5.62  | 125.93      | 119.92   |
| 1   | b     | 134 | ILE  | C-N-CA | 5.62  | 125.93      | 119.92   |
| 32  | H     | 89  | VAL  | N-CA-C | 5.62  | 118.92      | 111.17   |
| 3   | d     | 83  | VAL  | N-CA-C | 5.61  | 121.00      | 109.34   |
| 9   | j     | 109 | LEU  | N-CA-C | -5.60 | 103.01      | 110.07   |
| 31  | G     | 170 | ILE  | N-CA-C | -5.60 | 104.90      | 111.00   |
| 20  | u     | 82  | VAL  | N-CA-C | 5.60  | 116.65      | 108.53   |
| 44  | T     | 52  | ARG  | N-CA-C | -5.59 | 105.26      | 111.36   |
| 15  | p     | 109 | ILE  | N-CA-C | -5.58 | 102.02      | 108.82   |
| 45  | U     | 69  | ASP  | N-CA-C | 5.57  | 117.03      | 111.07   |
| 2   | c     | 50  | VAL  | N-CA-C | 5.55  | 115.60      | 108.82   |
| 6   | g     | 67  | ALA  | N-CA-C | -5.54 | 105.40      | 111.82   |
| 20  | u     | 25  | LYS  | N-CA-C | -5.54 | 106.45      | 113.43   |
| 4   | e     | 124 | ARG  | N-CA-C | -5.53 | 107.54      | 114.56   |
| 5   | f     | 94  | ARG  | N-CA-C | 5.52  | 118.66      | 110.48   |
| 15  | p     | 2   | ASN  | N-CA-C | -5.51 | 105.82      | 112.54   |
| 8   | i     | 73  | PRO  | CA-C-N | 5.50  | 125.51      | 119.90   |
| 8   | i     | 73  | PRO  | C-N-CA | 5.50  | 125.51      | 119.90   |
| 46  | V     | 30  | HIS  | CA-C-N | 5.49  | 126.70      | 119.84   |
| 46  | V     | 30  | HIS  | C-N-CA | 5.49  | 126.70      | 119.84   |
| 13  | n     | 11  | ASN  | N-CA-C | 5.48  | 119.00      | 111.54   |
| 24  | y     | 10  | SER  | N-CA-C | 5.47  | 117.68      | 111.11   |
| 21  | v     | 45  | ASP  | N-CA-C | 5.47  | 117.67      | 111.11   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | n     | 68   | ALA  | N-CA-C      | -5.47 | 105.87      | 112.54   |
| 17  | r     | 43   | ASN  | N-CA-C      | -5.46 | 105.73      | 112.72   |
| 11  | l     | 127  | VAL  | N-CA-C      | 5.46  | 116.64      | 109.21   |
| 29  | E     | 33   | THR  | N-CA-C      | 5.46  | 122.43      | 110.80   |
| 7   | h     | 51   | TYR  | N-CA-C      | 5.45  | 119.19      | 112.54   |
| 38  | N     | 126  | PHE  | N-CA-C      | 5.45  | 117.91      | 110.55   |
| 13  | n     | 44   | LEU  | N-CA-C      | -5.45 | 106.14      | 112.89   |
| 52  | 3     | 1190 | G    | C2'-C3'-O3' | 5.42  | 117.63      | 109.50   |
| 10  | k     | 67   | LYS  | N-CA-C      | -5.42 | 106.62      | 113.18   |
| 52  | 3     | 1300 | G    | N9-C1'-C2'  | 5.42  | 120.13      | 112.00   |
| 34  | J     | 135  | VAL  | N-CA-C      | 5.39  | 116.12      | 110.62   |
| 53  | 1     | 1020 | A    | C2'-C3'-O3' | 5.39  | 117.59      | 109.50   |
| 5   | f     | 148  | ARG  | N-CA-C      | -5.38 | 105.45      | 112.23   |
| 1   | b     | 39   | SER  | N-CA-C      | 5.38  | 118.06      | 111.82   |
| 6   | g     | 117  | LEU  | CA-C-N      | 5.37  | 124.56      | 118.97   |
| 6   | g     | 117  | LEU  | C-N-CA      | 5.37  | 124.56      | 118.97   |
| 31  | G     | 90   | PHE  | N-CA-C      | 5.33  | 117.28      | 109.24   |
| 43  | S     | 7    | ALA  | N-CA-C      | -5.33 | 105.64      | 111.82   |
| 13  | n     | 89   | SER  | N-CA-C      | 5.33  | 116.89      | 111.14   |
| 16  | q     | 59   | LEU  | N-CA-C      | -5.32 | 105.39      | 111.14   |
| 25  | z     | 42   | ALA  | N-CA-C      | -5.32 | 104.91      | 111.40   |
| 12  | m     | 118  | LYS  | N-CA-C      | -5.32 | 105.53      | 112.23   |
| 31  | G     | 111  | LYS  | N-CA-C      | -5.32 | 105.65      | 111.82   |
| 1   | b     | 153  | LEU  | N-CA-C      | 5.30  | 117.93      | 110.14   |
| 34  | J     | 87   | VAL  | N-CA-C      | 5.30  | 116.08      | 108.93   |
| 14  | o     | 25   | ARG  | N-CA-C      | 5.30  | 117.36      | 110.53   |
| 13  | n     | 53   | THR  | N-CA-C      | -5.29 | 105.59      | 111.36   |
| 37  | M     | 62   | LEU  | N-CA-C      | 5.28  | 118.34      | 110.52   |
| 5   | f     | 6    | ALA  | CA-C-N      | 5.28  | 126.44      | 119.84   |
| 5   | f     | 6    | ALA  | C-N-CA      | 5.28  | 126.44      | 119.84   |
| 33  | I     | 34   | GLU  | N-CA-C      | 5.28  | 122.04      | 110.80   |
| 32  | H     | 5    | HIS  | CA-C-N      | 5.27  | 126.42      | 119.84   |
| 32  | H     | 5    | HIS  | C-N-CA      | 5.27  | 126.42      | 119.84   |
| 39  | O     | 42   | LEU  | CA-C-N      | 5.27  | 126.42      | 119.84   |
| 39  | O     | 42   | LEU  | C-N-CA      | 5.27  | 126.42      | 119.84   |
| 31  | G     | 179  | GLY  | N-CA-C      | -5.26 | 107.38      | 116.01   |
| 16  | q     | 106  | THR  | N-CA-C      | 5.25  | 117.01      | 111.28   |
| 25  | z     | 51   | SER  | N-CA-C      | 5.25  | 120.03      | 111.37   |
| 42  | R     | 110  | GLY  | CA-C-N      | 5.25  | 125.16      | 119.76   |
| 42  | R     | 110  | GLY  | C-N-CA      | 5.25  | 125.16      | 119.76   |
| 22  | w     | 23   | GLY  | N-CA-C      | 5.24  | 117.96      | 111.93   |
| 33  | I     | 37   | PRO  | N-CA-C      | -5.24 | 106.90      | 114.18   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | n     | 48   | VAL  | N-CA-C      | 5.22  | 116.00      | 110.72   |
| 24  | y     | 27   | ASN  | N-CA-C      | 5.22  | 116.66      | 110.97   |
| 35  | K     | 68   | GLN  | N-CA-C      | 5.22  | 117.72      | 111.71   |
| 49  | Y     | 33   | LYS  | N-CA-C      | -5.21 | 105.68      | 111.36   |
| 3   | d     | 75   | SER  | CA-C-N      | 5.21  | 124.93      | 119.82   |
| 3   | d     | 75   | SER  | C-N-CA      | 5.21  | 124.93      | 119.82   |
| 33  | I     | 199  | ILE  | N-CA-C      | 5.20  | 115.92      | 110.62   |
| 34  | J     | 77   | ASN  | N-CA-C      | 5.19  | 118.75      | 111.90   |
| 10  | k     | 40   | LYS  | N-CA-C      | -5.19 | 102.00      | 110.20   |
| 5   | f     | 168  | VAL  | N-CA-C      | 5.18  | 116.18      | 108.46   |
| 42  | R     | 102  | LYS  | N-CA-C      | -5.18 | 106.22      | 112.54   |
| 4   | e     | 99   | PHE  | N-CA-C      | -5.17 | 105.82      | 111.82   |
| 24  | y     | 57   | LEU  | N-CA-C      | -5.16 | 105.73      | 111.36   |
| 1   | b     | 8    | THR  | N-CA-C      | -5.15 | 106.94      | 113.18   |
| 42  | R     | 74   | MET  | N-CA-C      | -5.14 | 105.36      | 111.69   |
| 33  | I     | 5    | GLY  | CA-C-N      | 5.14  | 126.26      | 119.84   |
| 33  | I     | 5    | GLY  | C-N-CA      | 5.14  | 126.26      | 119.84   |
| 36  | L     | 128  | GLU  | N-CA-C      | -5.13 | 106.80      | 113.16   |
| 24  | y     | 18   | LEU  | N-CA-C      | -5.13 | 106.28      | 112.54   |
| 39  | O     | 17   | LEU  | N-CA-C      | -5.12 | 107.10      | 113.55   |
| 50  | Z     | 58   | LYS  | N-CA-C      | -5.11 | 105.89      | 111.82   |
| 52  | 3     | 1201 | A    | C2'-C3'-O3' | 5.11  | 117.16      | 109.50   |
| 33  | I     | 91   | ALA  | N-CA-C      | -5.11 | 105.89      | 111.82   |
| 33  | I     | 172  | VAL  | N-CA-C      | 5.09  | 115.29      | 108.17   |
| 16  | q     | 85   | ALA  | N-CA-C      | -5.09 | 106.48      | 113.30   |
| 19  | t     | 20   | ALA  | N-CA-C      | -5.09 | 106.76      | 113.12   |
| 40  | P     | 117  | HIS  | N-CA-C      | -5.08 | 103.98      | 111.81   |
| 6   | g     | 108  | VAL  | N-CA-C      | 5.07  | 115.59      | 108.89   |
| 44  | T     | 62   | ARG  | N-CA-C      | -5.07 | 105.21      | 111.40   |
| 49  | Y     | 83   | ASN  | N-CA-C      | -5.07 | 106.60      | 112.89   |
| 8   | i     | 34   | ILE  | N-CA-C      | 5.06  | 115.78      | 110.62   |
| 31  | G     | 208  | ALA  | N-CA-C      | -5.06 | 105.85      | 112.23   |
| 5   | f     | 92   | GLY  | N-CA-C      | -5.05 | 108.27      | 115.64   |
| 32  | H     | 157  | GLY  | N-CA-C      | -5.05 | 108.35      | 115.32   |
| 31  | G     | 26   | MET  | N-CA-C      | -5.05 | 105.85      | 112.41   |
| 26  | B     | 19   | ASP  | N-CA-C      | -5.05 | 106.90      | 113.16   |
| 20  | u     | 89   | GLY  | N-CA-C      | -5.04 | 107.25      | 115.46   |
| 9   | j     | 29   | ALA  | N-CA-C      | 5.04  | 116.46      | 111.07   |
| 39  | O     | 44   | THR  | N-CA-C      | 5.03  | 117.81      | 109.46   |
| 40  | P     | 125  | LYS  | N-CA-C      | 5.03  | 117.76      | 110.17   |
| 32  | H     | 172  | VAL  | CA-C-N      | 5.02  | 126.12      | 119.84   |
| 32  | H     | 172  | VAL  | C-N-CA      | 5.02  | 126.12      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 21  | v     | 46  | LYS  | N-CA-C | 5.02  | 116.44      | 110.97   |
| 16  | q     | 70  | GLN  | N-CA-C | -5.01 | 106.68      | 112.89   |
| 49  | Y     | 48  | LYS  | N-CA-C | -5.01 | 105.73      | 111.14   |
| 24  | y     | 55  | THR  | N-CA-C | -5.01 | 105.73      | 111.14   |
| 32  | H     | 161 | ILE  | N-CA-C | 5.01  | 115.51      | 110.05   |
| 48  | X     | 34  | SER  | N-CA-C | 5.01  | 117.43      | 108.17   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | b     | 2083  | 0        | 2157     | 112     | 0            |
| 2   | c     | 1565  | 0        | 1616     | 63      | 0            |
| 3   | d     | 1552  | 0        | 1619     | 67      | 0            |
| 4   | e     | 1411  | 0        | 1447     | 54      | 0            |
| 5   | f     | 1323  | 0        | 1374     | 38      | 0            |
| 6   | g     | 1111  | 0        | 1148     | 56      | 0            |
| 7   | h     | 989   | 0        | 1025     | 60      | 0            |
| 8   | i     | 1032  | 0        | 1088     | 53      | 0            |
| 9   | j     | 1129  | 0        | 1162     | 38      | 0            |
| 10  | k     | 939   | 0        | 1012     | 45      | 0            |
| 11  | l     | 1045  | 0        | 1117     | 53      | 0            |
| 12  | m     | 1074  | 0        | 1157     | 56      | 0            |
| 13  | n     | 961   | 0        | 1000     | 29      | 0            |
| 14  | o     | 892   | 0        | 923      | 31      | 0            |
| 15  | p     | 917   | 0        | 965      | 35      | 0            |
| 16  | q     | 947   | 0        | 1022     | 43      | 0            |
| 17  | r     | 816   | 0        | 839      | 31      | 0            |
| 18  | s     | 857   | 0        | 922      | 33      | 0            |
| 19  | t     | 739   | 0        | 807      | 28      | 0            |
| 20  | u     | 780   | 0        | 834      | 46      | 0            |
| 21  | v     | 753   | 0        | 780      | 22      | 0            |
| 22  | w     | 575   | 0        | 592      | 25      | 0            |
| 23  | x     | 625   | 0        | 655      | 24      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 24  | y     | 509    | 0        | 543      | 15      | 0            |
| 25  | z     | 449    | 0        | 491      | 17      | 0            |
| 26  | B     | 444    | 0        | 461      | 17      | 0            |
| 27  | C     | 410    | 0        | 440      | 18      | 0            |
| 28  | D     | 377    | 0        | 418      | 26      | 0            |
| 29  | E     | 504    | 0        | 574      | 25      | 0            |
| 30  | F     | 302    | 0        | 343      | 10      | 0            |
| 31  | G     | 1757   | 0        | 1787     | 48      | 0            |
| 32  | H     | 1625   | 0        | 1699     | 68      | 0            |
| 33  | I     | 1643   | 0        | 1710     | 64      | 0            |
| 34  | J     | 1157   | 0        | 1199     | 58      | 0            |
| 35  | K     | 818    | 0        | 808      | 40      | 0            |
| 36  | L     | 1182   | 0        | 1240     | 46      | 0            |
| 37  | M     | 979    | 0        | 1034     | 54      | 0            |
| 38  | N     | 1022   | 0        | 1070     | 48      | 0            |
| 39  | O     | 787    | 0        | 828      | 41      | 0            |
| 40  | P     | 870    | 0        | 878      | 49      | 0            |
| 41  | Q     | 955    | 0        | 1019     | 49      | 0            |
| 42  | R     | 884    | 0        | 944      | 43      | 0            |
| 43  | S     | 805    | 0        | 847      | 42      | 0            |
| 44  | T     | 714    | 0        | 737      | 25      | 0            |
| 45  | U     | 649    | 0        | 666      | 33      | 0            |
| 46  | V     | 649    | 0        | 691      | 27      | 0            |
| 47  | W     | 536    | 0        | 552      | 20      | 0            |
| 48  | X     | 638    | 0        | 665      | 33      | 0            |
| 49  | Y     | 665    | 0        | 714      | 39      | 0            |
| 50  | Z     | 545    | 0        | 579      | 29      | 0            |
| 51  | a     | 1027   | 0        | 1092     | 45      | 0            |
| 52  | 3     | 33012  | 0        | 16618    | 454     | 0            |
| 53  | 1     | 62317  | 0        | 31346    | 876     | 0            |
| 54  | 2     | 2568   | 0        | 1303     | 54      | 0            |
| 55  | 5     | 1640   | 0        | 836      | 7       | 0            |
| 55  | 6     | 1640   | 0        | 837      | 18      | 0            |
| 56  | 4     | 388    | 0        | 197      | 9       | 0            |
| 57  | 7     | 1557   | 0        | 789      | 13      | 0            |
| 58  | 5     | 10     | 0        | 10       | 1       | 0            |
| All | All   | 150149 | 0        | 101226   | 2886    | 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 11.

All (2886) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:1:45:G:H5''   | 53:1:46:G:H5'    | 1.32                     | 1.05              |
| 4:e:25:MET:HE1   | 54:2:55:U:H1'    | 1.40                     | 1.03              |
| 11:l:47:ARG:HH11 | 53:1:195:A:H5''  | 1.30                     | 0.97              |
| 37:M:21:LYS:HE3  | 52:3:827:U:H5''  | 1.48                     | 0.96              |
| 10:k:48:PRO:HG3  | 52:3:1422:G:H5'  | 1.48                     | 0.96              |
| 32:H:162:ALA:HB2 | 52:3:1056:U:H5'  | 1.48                     | 0.95              |
| 8:i:123:ALA:HB1  | 53:1:1081:U:H4'  | 1.49                     | 0.94              |
| 53:1:1906:G:H2'  | 53:1:1907:G:H5'' | 1.49                     | 0.93              |
| 11:l:47:ARG:HH12 | 53:1:196:A:H5''  | 1.33                     | 0.93              |
| 9:j:81:ILE:HG23  | 9:j:82:GLY:H     | 1.35                     | 0.92              |
| 10:k:43:ILE:HD11 | 10:k:46:ALA:HB2  | 1.52                     | 0.91              |
| 16:q:61:ILE:HG21 | 53:1:1009:A:H4'  | 1.52                     | 0.90              |
| 46:V:25:GLU:HB3  | 46:V:38:LYS:HD2  | 1.53                     | 0.90              |
| 8:i:25:PRO:HB2   | 53:1:1095:A:H61  | 1.38                     | 0.88              |
| 42:R:113:LYS:HG3 | 42:R:114:PRO:HD3 | 1.56                     | 0.87              |
| 6:g:97:ARG:HH22  | 53:1:2220:U:H5'  | 1.38                     | 0.87              |
| 33:I:6:PRO:HG3   | 52:3:430:A:H4'   | 1.55                     | 0.86              |
| 6:g:55:GLU:HA    | 6:g:58:LEU:HD13  | 1.58                     | 0.85              |
| 53:1:1801:A:H5'' | 53:1:2203:U:H2'  | 1.59                     | 0.84              |
| 55:5:13:C:H2'    | 55:5:14:A:H5''   | 1.57                     | 0.84              |
| 49:Y:28:ARG:NH2  | 52:3:1437:A:H5'' | 1.93                     | 0.84              |
| 1:b:7:PRO:O      | 53:1:1695:G:H1'  | 1.78                     | 0.84              |
| 55:5:57:A:H2'    | 55:5:58:A:H5'    | 1.59                     | 0.84              |
| 53:1:1053:C:H2'  | 53:1:1054:A:H5'' | 1.58                     | 0.83              |
| 11:l:79:LEU:HD12 | 11:l:114:GLY:H   | 1.41                     | 0.83              |
| 42:R:97:ARG:HB2  | 42:R:99:GLN:HE22 | 1.42                     | 0.83              |
| 1:b:131:MET:HE2  | 1:b:187:CYS:HB2  | 1.58                     | 0.83              |
| 47:W:59:LYS:HD3  | 52:3:734:G:O2'   | 1.79                     | 0.83              |
| 53:1:1020:A:H1'  | 53:1:1021:A:OP2  | 1.77                     | 0.83              |
| 33:I:54:LEU:HD21 | 52:3:509:A:H4'   | 1.61                     | 0.83              |
| 9:j:78:THR:HG23  | 9:j:80:HIS:H     | 1.43                     | 0.83              |
| 36:L:27:ASN:HD22 | 52:3:1374:A:H4'  | 1.42                     | 0.82              |
| 11:l:67:THR:HG21 | 53:1:244:A:H5''  | 1.61                     | 0.82              |
| 22:w:17:LEU:HD13 | 22:w:37:ARG:HB2  | 1.62                     | 0.82              |
| 52:3:1306:A:H61  | 52:3:1331:G:H1'  | 1.45                     | 0.82              |
| 6:g:97:ARG:HH22  | 53:1:2220:U:C5'  | 1.92                     | 0.82              |
| 19:t:61:LEU:HD13 | 53:1:1340:U:H2'  | 1.62                     | 0.82              |
| 45:U:8:ARG:HB3   | 45:U:28:ARG:HD2  | 1.61                     | 0.82              |
| 53:1:572:A:H61   | 53:1:2029:G:H21  | 1.26                     | 0.82              |
| 9:j:96:ARG:HH11  | 53:1:2639:A:H5'' | 1.45                     | 0.81              |
| 18:s:93:ALA:HB2  | 53:1:1614:A:N1   | 1.95                     | 0.81              |
| 12:m:12:MET:HA   | 53:1:910:A:H62   | 1.45                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:R:100:ARG:HH21 | 42:R:102:LYS:HD2  | 1.46                     | 0.81              |
| 10:k:26:GLY:HA2   | 53:1:2563:U:H5''  | 1.60                     | 0.81              |
| 51:a:174:THR:HB   | 53:1:2124:G:H5''  | 1.62                     | 0.81              |
| 9:j:13:ARG:HD2    | 9:j:121:LYS:HE2   | 1.61                     | 0.81              |
| 34:J:54:GLU:HG2   | 34:J:56:PRO:HD2   | 1.61                     | 0.81              |
| 7:h:34:THR:HG21   | 53:1:1057:A:H1'   | 1.61                     | 0.80              |
| 7:h:55:VAL:HA     | 53:1:1084:A:H4'   | 1.64                     | 0.80              |
| 21:v:49:ASN:ND2   | 53:1:1040:A:H5'   | 1.97                     | 0.80              |
| 31:G:206:ILE:H    | 31:G:206:ILE:HD12 | 1.45                     | 0.80              |
| 13:n:100:CYS:HA   | 26:B:42:ILE:HG12  | 1.62                     | 0.79              |
| 22:w:38:GLY:HA2   | 53:1:2330:G:H21   | 1.46                     | 0.79              |
| 53:1:2286:G:H5''  | 53:1:2287:A:OP1   | 1.82                     | 0.79              |
| 49:Y:24:ARG:HA    | 49:Y:27:MET:HE3   | 1.64                     | 0.79              |
| 32:H:171:ARG:HG3  | 52:3:1106:G:H5''  | 1.64                     | 0.79              |
| 45:U:46:LYS:HE2   | 52:3:617:G:H4'    | 1.65                     | 0.79              |
| 34:J:123:LEU:HD11 | 52:3:7:A:H2'      | 1.65                     | 0.78              |
| 41:Q:29:LYS:HD3   | 52:3:363:A:OP1    | 1.83                     | 0.78              |
| 53:1:119:A:H4'    | 53:1:120:U:H5'    | 1.64                     | 0.78              |
| 20:u:36:GLU:HA    | 20:u:61:GLU:HG2   | 1.64                     | 0.78              |
| 51:a:218:MET:HE1  | 53:1:2128:G:H4'   | 1.65                     | 0.78              |
| 12:m:23:GLY:HA3   | 12:m:66:ARG:HH22  | 1.47                     | 0.78              |
| 31:G:18:GLN:HG3   | 31:G:20:ARG:H     | 1.48                     | 0.78              |
| 8:i:93:ASN:OD1    | 53:1:1077:A:H5'   | 1.83                     | 0.78              |
| 4:e:25:MET:CE     | 54:2:55:U:H1'     | 2.13                     | 0.78              |
| 52:3:405:U:H3'    | 52:3:406:G:H5'    | 1.64                     | 0.78              |
| 50:Z:9:GLU:HB3    | 50:Z:10:PRO:HD3   | 1.63                     | 0.77              |
| 1:b:160:TYR:HB3   | 1:b:193:GLU:HG2   | 1.66                     | 0.77              |
| 9:j:26:GLY:HA3    | 53:1:1140:C:H5'   | 1.66                     | 0.77              |
| 9:j:58:ASN:HB3    | 9:j:61:LYS:HB2    | 1.66                     | 0.77              |
| 48:X:38:THR:HA    | 48:X:69:LYS:HA    | 1.66                     | 0.77              |
| 52:3:484:G:H4'    | 52:3:485:U:H5''   | 1.65                     | 0.77              |
| 3:d:117:ARG:HH12  | 11:l:2:ARG:HH21   | 1.32                     | 0.77              |
| 19:t:59:ASN:HB2   | 19:t:84:TYR:HB2   | 1.66                     | 0.77              |
| 3:d:69:ARG:HH12   | 53:1:2060:A:H62   | 1.33                     | 0.77              |
| 11:l:47:ARG:HG2   | 11:l:50:PHE:HB2   | 1.67                     | 0.77              |
| 6:g:73:ASN:O      | 6:g:76:GLU:HG3    | 1.84                     | 0.76              |
| 28:D:11:LYS:HE3   | 53:1:686:U:H5''   | 1.67                     | 0.76              |
| 53:1:2391:G:H4'   | 53:1:2392:A:OP1   | 1.85                     | 0.76              |
| 53:1:2296:U:H5''  | 53:1:2297:A:OP1   | 1.86                     | 0.76              |
| 15:p:88:ARG:HE    | 15:p:112:ARG:HB3  | 1.51                     | 0.76              |
| 40:P:74:LYS:HD3   | 40:P:77:GLY:HA2   | 1.68                     | 0.76              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:b:43:ASN:HD21  | 1:b:45:ASN:HB2    | 1.51                     | 0.75              |
| 9:j:95:ARG:HG2   | 9:j:96:ARG:HD2    | 1.66                     | 0.75              |
| 13:n:69:ARG:O    | 13:n:70:THR:HG22  | 1.87                     | 0.75              |
| 21:v:64:VAL:HG22 | 21:v:69:GLU:HG3   | 1.69                     | 0.75              |
| 31:G:20:ARG:HG3  | 52:3:831:A:H5'    | 1.68                     | 0.75              |
| 15:p:52:ARG:HB2  | 15:p:55:HIS:HB2   | 1.66                     | 0.75              |
| 2:c:149:ASN:HB3  | 53:1:2572:A:OP2   | 1.88                     | 0.74              |
| 6:g:8:LYS:HD2    | 6:g:9:VAL:N       | 2.02                     | 0.74              |
| 52:3:1201:A:H1'  | 52:3:1202:U:OP2   | 1.86                     | 0.74              |
| 53:1:1906:G:C2'  | 53:1:1907:G:H5''  | 2.18                     | 0.74              |
| 53:1:2427:C:H5'' | 53:1:2429:G:H5'   | 1.69                     | 0.74              |
| 25:z:47:ILE:HG23 | 25:z:56:VAL:HG21  | 1.70                     | 0.74              |
| 40:P:34:THR:HA   | 40:P:40:ALA:HA    | 1.69                     | 0.74              |
| 53:1:1664:A:H61  | 53:1:1996:C:H42   | 1.35                     | 0.74              |
| 52:3:1158:C:H2'  | 52:3:1159:U:H4'   | 1.69                     | 0.74              |
| 7:h:58:THR:HG23  | 53:1:1107:G:H5'   | 1.70                     | 0.73              |
| 22:w:68:LYS:HE2  | 54:2:11:C:OP1     | 1.88                     | 0.73              |
| 33:I:104:MET:HE1 | 33:I:172:VAL:HG13 | 1.70                     | 0.73              |
| 51:a:11:ILE:HG23 | 51:a:33:LEU:HD22  | 1.69                     | 0.73              |
| 52:3:1259:C:H3'  | 52:3:1260:G:H5''  | 1.69                     | 0.73              |
| 44:T:61:GLN:O    | 44:T:65:LEU:HG    | 1.87                     | 0.73              |
| 40:P:15:VAL:HG22 | 40:P:16:SER:H     | 1.53                     | 0.73              |
| 1:b:132:ARG:HD3  | 6:g:123:ARG:HH21  | 1.53                     | 0.73              |
| 38:N:35:GLU:HA   | 38:N:39:GLY:HA3   | 1.68                     | 0.73              |
| 23:x:56:ARG:HH12 | 53:1:399:U:H5''   | 1.53                     | 0.73              |
| 33:I:119:HIS:CG  | 52:3:438:U:H4'    | 2.24                     | 0.73              |
| 48:X:30:LEU:H    | 48:X:30:LEU:HD12  | 1.52                     | 0.73              |
| 51:a:206:GLY:HA2 | 53:1:1860:G:H5''  | 1.70                     | 0.73              |
| 2:c:151:THR:HB   | 2:c:152:PRO:HD3   | 1.71                     | 0.73              |
| 5:f:132:LEU:HD23 | 5:f:132:LEU:H     | 1.53                     | 0.73              |
| 16:q:65:ASN:HD21 | 16:q:69:ARG:HE    | 1.36                     | 0.73              |
| 23:x:56:ARG:HH22 | 53:1:399:U:P      | 2.12                     | 0.73              |
| 30:F:31:PRO:HB3  | 53:1:2527:C:H5''  | 1.70                     | 0.73              |
| 1:b:267:VAL:HG12 | 1:b:268:ARG:HD2   | 1.70                     | 0.73              |
| 38:N:46:VAL:HA   | 38:N:49:GLN:HG3   | 1.71                     | 0.73              |
| 11:l:79:LEU:HD11 | 11:l:112:LEU:HD12 | 1.71                     | 0.72              |
| 32:H:55:VAL:HB   | 32:H:66:THR:HB    | 1.71                     | 0.72              |
| 53:1:2277:G:H2'  | 53:1:2278:A:H5''  | 1.70                     | 0.72              |
| 7:h:58:THR:HG23  | 53:1:1107:G:C5'   | 2.18                     | 0.72              |
| 31:G:89:PHE:HB3  | 31:G:150:ILE:HG22 | 1.69                     | 0.72              |
| 28:D:24:THR:HG23 | 28:D:27:GLY:H     | 1.55                     | 0.72              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:b:200:MET:HE3   | 52:3:773:G:H4'   | 1.70                     | 0.72              |
| 53:1:275:C:H2'    | 53:1:276:U:H4'   | 1.70                     | 0.72              |
| 52:3:1500:A:H5''  | 52:3:1508:A:H5'' | 1.72                     | 0.72              |
| 44:T:49:HIS:HA    | 44:T:52:ARG:HB2  | 1.72                     | 0.72              |
| 53:1:475:C:H4'    | 53:1:510:C:H5'   | 1.71                     | 0.71              |
| 3:d:63:LYS:HD2    | 53:1:2444:G:OP2  | 1.90                     | 0.71              |
| 5:f:25:ILE:HD12   | 5:f:74:MET:HB3   | 1.70                     | 0.71              |
| 12:m:69:PRO:HA    | 12:m:94:ALA:HB2  | 1.73                     | 0.71              |
| 32:H:162:ALA:HB2  | 52:3:1056:U:C5'  | 2.19                     | 0.71              |
| 51:a:170:ILE:HG21 | 53:1:2177:C:H1'  | 1.69                     | 0.71              |
| 1:b:23:LEU:HD11   | 1:b:82:TYR:HB2   | 1.71                     | 0.71              |
| 31:G:131:LYS:HE2  | 52:3:1160:G:OP1  | 1.89                     | 0.71              |
| 8:i:3:LYS:HG2     | 8:i:4:VAL:H      | 1.56                     | 0.71              |
| 33:I:103:ARG:HH22 | 33:I:164:ARG:HB3 | 1.56                     | 0.71              |
| 3:d:84:THR:HG23   | 53:1:801:G:H1    | 1.53                     | 0.71              |
| 7:h:37:LYS:HG3    | 7:h:41:LEU:HD12  | 1.70                     | 0.71              |
| 50:Z:48:LYS:HE2   | 52:3:724:G:OP1   | 1.91                     | 0.71              |
| 52:3:1496:C:H1'   | 52:3:1517:G:H22  | 1.55                     | 0.71              |
| 10:k:48:PRO:CG    | 52:3:1422:G:H5'  | 2.20                     | 0.70              |
| 17:r:63:VAL:HG12  | 17:r:96:VAL:HG12 | 1.73                     | 0.70              |
| 2:c:154:LYS:HD3   | 53:1:2024:G:H4'  | 1.72                     | 0.70              |
| 31:G:25:LYS:HD2   | 31:G:191:ASP:OD1 | 1.90                     | 0.70              |
| 53:1:49:A:H5'     | 53:1:51:G:O4'    | 1.91                     | 0.70              |
| 1:b:165:ALA:H     | 1:b:172:THR:HB   | 1.56                     | 0.70              |
| 11:l:38:GLN:HB3   | 53:1:832:U:H5'   | 1.73                     | 0.70              |
| 42:R:16:ILE:HD11  | 52:3:1302:C:OP2  | 1.91                     | 0.70              |
| 1:b:91:ALA:HB2    | 1:b:105:ALA:HB2  | 1.73                     | 0.70              |
| 34:J:111:ARG:HD2  | 34:J:112:ALA:N   | 2.07                     | 0.70              |
| 2:c:148:GLN:HB2   | 2:c:152:PRO:HG2  | 1.74                     | 0.70              |
| 1:b:153:LEU:HD22  | 53:1:1799:G:H21  | 1.57                     | 0.70              |
| 16:q:61:ILE:CG2   | 53:1:1009:A:H4'  | 2.22                     | 0.70              |
| 53:1:1300:G:H4'   | 53:1:1301:A:H5'  | 1.74                     | 0.70              |
| 20:u:90:LYS:HE2   | 53:1:101:A:H61   | 1.55                     | 0.70              |
| 4:e:63:LYS:O      | 54:2:42:C:H1'    | 1.92                     | 0.69              |
| 41:Q:43:LYS:HZ1   | 56:4:20:U:H4'    | 1.57                     | 0.69              |
| 52:3:1306:A:N6    | 52:3:1331:G:H1'  | 2.07                     | 0.69              |
| 2:c:55:LYS:HG3    | 2:c:77:ARG:HA    | 1.74                     | 0.69              |
| 14:o:81:ARG:O     | 14:o:84:GLU:HG2  | 1.92                     | 0.69              |
| 3:d:52:VAL:HG13   | 53:1:452:G:OP1   | 1.93                     | 0.69              |
| 25:z:29:ARG:NE    | 53:1:1183:U:H5'' | 2.07                     | 0.69              |
| 40:P:78:ILE:HD11  | 40:P:81:LEU:HB3  | 1.74                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:b:153:LEU:HD22 | 53:1:1799:G:N2    | 2.08                     | 0.69              |
| 21:v:70:ILE:H    | 21:v:70:ILE:HD12  | 1.57                     | 0.69              |
| 41:Q:43:LYS:NZ   | 56:4:20:U:H4'     | 2.07                     | 0.69              |
| 4:e:23:SER:H     | 4:e:26:GLN:NE2    | 1.90                     | 0.69              |
| 11:l:38:GLN:HE22 | 11:l:45:GLY:H     | 1.39                     | 0.69              |
| 22:w:33:ILE:HG22 | 22:w:34:VAL:HG23  | 1.75                     | 0.69              |
| 43:S:33:VAL:HG21 | 52:3:1272:G:H5'   | 1.74                     | 0.69              |
| 16:q:12:ARG:HH12 | 53:1:812:C:H4'    | 1.58                     | 0.69              |
| 4:e:111:ARG:HH12 | 4:e:132:ARG:HD2   | 1.58                     | 0.69              |
| 7:h:48:ALA:HB3   | 7:h:51:TYR:HE1    | 1.57                     | 0.69              |
| 12:m:34:LYS:HE3  | 12:m:131:VAL:HG11 | 1.75                     | 0.69              |
| 13:n:10:LEU:HD21 | 13:n:40:LYS:HG2   | 1.74                     | 0.69              |
| 43:S:36:SER:HA   | 43:S:40:ARG:HD3   | 1.75                     | 0.69              |
| 46:V:57:VAL:HG23 | 46:V:78:VAL:HG13  | 1.75                     | 0.69              |
| 49:Y:28:ARG:HD3  | 52:3:1438:G:OP1   | 1.92                     | 0.69              |
| 3:d:191:ASP:HA   | 3:d:194:LYS:HD2   | 1.75                     | 0.68              |
| 6:g:94:ILE:HD11  | 6:g:122:LEU:HD23  | 1.74                     | 0.68              |
| 38:N:51:LEU:HB3  | 38:N:56:MET:HG2   | 1.76                     | 0.68              |
| 52:3:208:U:H2'   | 52:3:210:C:H1'    | 1.75                     | 0.68              |
| 10:k:8:LEU:HB2   | 10:k:19:VAL:HG23  | 1.74                     | 0.68              |
| 10:k:66:LYS:HE3  | 53:1:1665:A:H5''  | 1.75                     | 0.68              |
| 7:h:102:ALA:HA   | 7:h:105:LYS:HE2   | 1.75                     | 0.68              |
| 15:p:111:GLU:HB3 | 15:p:113:LEU:HD22 | 1.74                     | 0.68              |
| 35:K:10:VAL:HG12 | 35:K:58:HIS:HB3   | 1.73                     | 0.68              |
| 52:3:516:U:H3    | 52:3:533:A:H62    | 1.39                     | 0.68              |
| 4:e:73:VAL:HG22  | 4:e:75:GLY:H      | 1.58                     | 0.68              |
| 42:R:44:ILE:H    | 42:R:44:ILE:HD12  | 1.58                     | 0.68              |
| 2:c:4:LEU:HD22   | 2:c:32:ASN:HD22   | 1.59                     | 0.68              |
| 20:u:73:ASN:HD21 | 20:u:75:ALA:HB3   | 1.58                     | 0.68              |
| 52:3:327:A:O2'   | 52:3:328:C:H4'    | 1.94                     | 0.68              |
| 54:2:3:C:H3'     | 54:2:4:C:H5''     | 1.75                     | 0.68              |
| 57:7:7:A:H3'     | 57:7:8:U:H5''     | 1.75                     | 0.68              |
| 4:e:25:MET:HE1   | 54:2:55:U:C1'     | 2.20                     | 0.68              |
| 53:1:546:U:H2'   | 53:1:547:A:H4'    | 1.75                     | 0.68              |
| 32:H:78:LYS:O    | 32:H:79:LYS:HG3   | 1.94                     | 0.68              |
| 45:U:7:ALA:HB3   | 45:U:18:GLN:HB2   | 1.74                     | 0.68              |
| 10:k:26:GLY:HA2  | 53:1:2563:U:C5'   | 2.22                     | 0.68              |
| 11:l:135:ILE:HB  | 11:l:142:ILE:HD11 | 1.76                     | 0.68              |
| 27:C:20:TYR:OH   | 53:1:2348:U:H5'   | 1.93                     | 0.68              |
| 21:v:51:GLN:HE22 | 21:v:86:LEU:HD21  | 1.59                     | 0.68              |
| 31:G:53:LEU:HD21 | 31:G:216:VAL:HG12 | 1.75                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 37:M:24:VAL:HB   | 37:M:60:LEU:HB2   | 1.75                     | 0.68              |
| 8:i:13:ALA:HA    | 8:i:53:PRO:HA     | 1.75                     | 0.68              |
| 11:l:36:LYS:HD2  | 53:1:807:U:OP2    | 1.94                     | 0.67              |
| 2:c:173:GLN:OE1  | 53:1:2731:G:H4'   | 1.94                     | 0.67              |
| 36:L:27:ASN:ND2  | 52:3:1374:A:H4'   | 2.08                     | 0.67              |
| 37:M:83:ARG:NH2  | 52:3:644:U:H5'    | 2.10                     | 0.67              |
| 43:S:7:ALA:O     | 43:S:10:VAL:HG12  | 1.94                     | 0.67              |
| 10:k:63:VAL:HG13 | 10:k:64:ARG:H     | 1.57                     | 0.67              |
| 32:H:87:ARG:HE   | 32:H:88:LYS:HZ2   | 1.43                     | 0.67              |
| 39:O:20:GLN:O    | 39:O:24:GLU:HG3   | 1.95                     | 0.67              |
| 2:c:131:ASP:HA   | 53:1:1994:C:OP1   | 1.94                     | 0.67              |
| 45:U:20:VAL:HG12 | 45:U:35:ARG:HA    | 1.76                     | 0.67              |
| 53:1:2055:C:H2'  | 53:1:2504:U:H5'   | 1.75                     | 0.67              |
| 15:p:108:ARG:HD2 | 52:3:1463:U:OP1   | 1.95                     | 0.67              |
| 4:e:87:LYS:HD3   | 53:1:2313:C:H4'   | 1.77                     | 0.67              |
| 34:J:24:VAL:HG22 | 34:J:25:LYS:H     | 1.60                     | 0.67              |
| 37:M:12:ARG:CZ   | 52:3:826:C:H5'    | 2.24                     | 0.67              |
| 41:Q:119:LYS:HG2 | 52:3:36:C:H5''    | 1.76                     | 0.67              |
| 53:1:2553:G:H3'  | 53:1:2554:U:H5''  | 1.76                     | 0.67              |
| 20:u:85:ARG:HG3  | 20:u:92:VAL:HG23  | 1.76                     | 0.67              |
| 32:H:149:LYS:HB2 | 32:H:172:VAL:HG11 | 1.75                     | 0.67              |
| 8:i:102:ARG:HH12 | 8:i:106:GLN:HB2   | 1.60                     | 0.67              |
| 28:D:34:ARG:HD3  | 53:1:467:G:OP2    | 1.95                     | 0.67              |
| 36:L:85:GLN:HB2  | 36:L:147:ASN:HD22 | 1.60                     | 0.67              |
| 54:2:3:C:C3'     | 54:2:4:C:H5''     | 2.25                     | 0.67              |
| 1:b:36:ASN:HB2   | 1:b:61:TYR:HB2    | 1.77                     | 0.66              |
| 35:K:38:ARG:HD3  | 35:K:97:THR:HA    | 1.77                     | 0.66              |
| 12:m:59:ARG:H    | 12:m:59:ARG:HD2   | 1.60                     | 0.66              |
| 17:r:76:LYS:HB2  | 17:r:85:LYS:HB3   | 1.76                     | 0.66              |
| 6:g:41:LYS:H     | 6:g:41:LYS:HD3    | 1.60                     | 0.66              |
| 29:E:51:LYS:HE2  | 53:1:937:C:H5''   | 1.77                     | 0.66              |
| 31:G:59:ILE:H    | 31:G:59:ILE:HD12  | 1.60                     | 0.66              |
| 49:Y:28:ARG:HH22 | 52:3:1437:A:H5''  | 1.58                     | 0.66              |
| 3:d:18:THR:HG23  | 3:d:19:PHE:HD1    | 1.60                     | 0.66              |
| 5:f:41:GLU:HA    | 5:f:54:ARG:HH21   | 1.61                     | 0.66              |
| 8:i:77:VAL:HA    | 8:i:80:LYS:HE2    | 1.76                     | 0.66              |
| 36:L:24:LYS:HE3  | 52:3:1375:A:H5''  | 1.78                     | 0.66              |
| 7:h:33:VAL:HG12  | 7:h:34:THR:H      | 1.60                     | 0.66              |
| 40:P:15:VAL:HG12 | 40:P:76:TYR:HB3   | 1.77                     | 0.66              |
| 41:Q:29:LYS:HA   | 52:3:363:A:OP1    | 1.95                     | 0.66              |
| 36:L:83:THR:HB   | 55:6:33:U:H4'     | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 37:M:113:ARG:HA  | 37:M:116:ARG:HE  | 1.60                     | 0.66              |
| 43:S:15:LEU:HD23 | 43:S:53:ASP:HB3  | 1.78                     | 0.66              |
| 54:2:3:C:H2'     | 54:2:4:C:H5''    | 1.78                     | 0.66              |
| 9:j:81:ILE:HG23  | 9:j:82:GLY:N     | 2.10                     | 0.66              |
| 36:L:109:LYS:HG3 | 36:L:110:ARG:H   | 1.61                     | 0.66              |
| 52:3:1200:C:H5'' | 52:3:1201:A:H3'  | 1.78                     | 0.66              |
| 53:1:161:A:H62   | 53:1:165:A:H61   | 1.42                     | 0.66              |
| 53:1:310:A:O2'   | 53:1:311:A:H5''  | 1.96                     | 0.66              |
| 53:1:1645:G:H5'' | 53:1:1646:C:H5'  | 1.78                     | 0.66              |
| 1:b:216:ARG:HH22 | 53:1:690:G:H4'   | 1.61                     | 0.65              |
| 8:i:20:SER:HB3   | 8:i:21:PRO:HD3   | 1.77                     | 0.65              |
| 39:O:30:LYS:HE2  | 39:O:36:VAL:HG22 | 1.77                     | 0.65              |
| 40:P:123:PRO:HG3 | 52:3:779:C:H5''  | 1.78                     | 0.65              |
| 42:R:25:GLY:H    | 52:3:1329:A:H5'' | 1.60                     | 0.65              |
| 53:1:776:G:H22   | 53:1:2072:C:H5'  | 1.61                     | 0.65              |
| 53:1:1133:A:H4'  | 53:1:1134:A:H5'' | 1.78                     | 0.65              |
| 5:f:65:GLY:HA3   | 53:1:2748:A:O2'  | 1.97                     | 0.65              |
| 8:i:29:GLN:HE21  | 8:i:30:GLN:HE22  | 1.44                     | 0.65              |
| 20:u:6:ARG:HH22  | 53:1:98:G:H1     | 1.42                     | 0.65              |
| 1:b:222:THR:HG23 | 53:1:1826:G:OP1  | 1.96                     | 0.65              |
| 24:y:2:LYS:HD2   | 53:1:78:U:OP2    | 1.95                     | 0.65              |
| 53:1:821:A:H5''  | 53:1:822:G:C5'   | 2.27                     | 0.65              |
| 3:d:84:THR:HG23  | 53:1:801:G:N1    | 2.11                     | 0.65              |
| 3:d:109:LEU:HD13 | 3:d:112:LEU:HD12 | 1.77                     | 0.65              |
| 6:g:30:LEU:HD13  | 6:g:36:ALA:HB3   | 1.78                     | 0.65              |
| 37:M:88:LYS:HE3  | 37:M:119:GLY:HA2 | 1.79                     | 0.65              |
| 7:h:10:ALA:O     | 7:h:14:GLU:HG3   | 1.97                     | 0.65              |
| 14:o:41:ALA:HB2  | 14:o:48:LEU:HD23 | 1.77                     | 0.65              |
| 19:t:14:PRO:HD3  | 24:y:30:MET:HG3  | 1.79                     | 0.65              |
| 20:u:64:ILE:HG12 | 20:u:68:ASN:HD21 | 1.60                     | 0.65              |
| 33:I:50:TYR:HD2  | 52:3:509:A:H5'   | 1.60                     | 0.65              |
| 50:Z:44:ARG:HD2  | 50:Z:47:ALA:HB3  | 1.78                     | 0.65              |
| 17:r:78:ARG:HH12 | 53:1:990:A:N6    | 1.94                     | 0.65              |
| 51:a:206:GLY:CA  | 53:1:1860:G:H5'' | 2.26                     | 0.65              |
| 43:S:45:LEU:HD11 | 48:X:10:ILE:HG13 | 1.78                     | 0.65              |
| 44:T:4:THR:HG23  | 52:3:659:U:H5''  | 1.79                     | 0.65              |
| 53:1:1053:C:C2'  | 53:1:1054:A:H5'' | 2.26                     | 0.65              |
| 1:b:216:ARG:NH2  | 53:1:690:G:H4'   | 2.12                     | 0.65              |
| 32:H:19:SER:O    | 43:S:93:PRO:HG3  | 1.97                     | 0.65              |
| 52:3:769:G:H4'   | 52:3:1513:A:H4'  | 1.79                     | 0.65              |
| 53:1:2584:U:H2'  | 53:1:2585:U:H2'  | 1.78                     | 0.65              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:c:48:ILE:HG22   | 2:c:82:PHE:HB2   | 1.78                     | 0.64              |
| 27:C:33:LEU:HD12  | 27:C:50:GLU:HB2  | 1.77                     | 0.64              |
| 53:1:729:G:H4'    | 53:1:763:G:H5'   | 1.79                     | 0.64              |
| 49:Y:25:SER:HA    | 49:Y:28:ARG:HD2  | 1.78                     | 0.64              |
| 53:1:310:A:C2'    | 53:1:311:A:H5''  | 2.28                     | 0.64              |
| 53:1:2048:G:C3'   | 53:1:2049:G:H5'' | 2.27                     | 0.64              |
| 12:m:8:LYS:HD2    | 53:1:869:G:H1'   | 1.78                     | 0.64              |
| 36:L:4:ARG:HD2    | 36:L:4:ARG:N     | 2.13                     | 0.64              |
| 20:u:73:ASN:ND2   | 20:u:75:ALA:HB3  | 2.12                     | 0.64              |
| 33:I:67:LEU:HB2   | 33:I:70:GLN:HG3  | 1.79                     | 0.64              |
| 4:e:107:VAL:HG12  | 4:e:108:PRO:HD3  | 1.79                     | 0.64              |
| 7:h:117:LEU:O     | 7:h:118:ILE:HG13 | 1.98                     | 0.64              |
| 11:l:63:LYS:HB3   | 29:E:12:ARG:HG2  | 1.78                     | 0.64              |
| 13:n:63:ARG:NH2   | 53:1:1454:C:H5'  | 2.12                     | 0.64              |
| 22:w:51:ARG:HH12  | 53:1:2387:U:P    | 2.21                     | 0.64              |
| 26:B:14:MET:HG2   | 53:1:15:G:O2'    | 1.97                     | 0.64              |
| 33:I:119:HIS:ND1  | 52:3:438:U:H4'   | 2.13                     | 0.64              |
| 57:7:44:G:H3'     | 57:7:45:U:H5''   | 1.80                     | 0.64              |
| 15:p:24:THR:HB    | 15:p:87:ARG:H    | 1.62                     | 0.64              |
| 33:I:80:ARG:HB2   | 52:3:613:C:OP1   | 1.97                     | 0.64              |
| 13:n:63:ARG:HH22  | 53:1:1454:C:H5'  | 1.63                     | 0.64              |
| 36:L:101:ARG:HH12 | 52:3:939:G:H5'   | 1.63                     | 0.64              |
| 3:d:52:VAL:HB     | 3:d:74:LYS:HE3   | 1.79                     | 0.63              |
| 7:h:59:LEU:HD21   | 53:1:1047:G:H8   | 1.61                     | 0.63              |
| 38:N:91:GLU:HA    | 38:N:94:ARG:HB2  | 1.79                     | 0.63              |
| 39:O:40:ILE:HB    | 39:O:73:LEU:HB2  | 1.79                     | 0.63              |
| 52:3:1379:G:O2'   | 52:3:1380:U:H5'  | 1.98                     | 0.63              |
| 41:Q:122:LYS:HD3  | 41:Q:122:LYS:N   | 2.13                     | 0.63              |
| 9:j:37:ARG:HG2    | 9:j:44:TYR:HE1   | 1.62                     | 0.63              |
| 53:1:542:C:H2'    | 53:1:543:G:H5''  | 1.80                     | 0.63              |
| 53:1:745:G:O2'    | 53:1:748:G:H1'   | 1.98                     | 0.63              |
| 32:H:21:TRP:HA    | 39:O:95:GLY:HA2  | 1.80                     | 0.63              |
| 32:H:162:ALA:CB   | 52:3:1056:U:H5'  | 2.26                     | 0.63              |
| 43:S:25:GLU:HB2   | 43:S:29:ILE:HD12 | 1.80                     | 0.63              |
| 52:3:1301:U:O2    | 52:3:1301:U:H2'  | 1.99                     | 0.63              |
| 12:m:45:GLN:HE21  | 53:1:2485:G:H5'' | 1.62                     | 0.63              |
| 22:w:35:ARG:HA    | 22:w:54:THR:HG23 | 1.79                     | 0.63              |
| 53:1:1322:A:H61   | 53:1:1333:G:H21  | 1.46                     | 0.63              |
| 53:1:1415:U:H2'   | 53:1:1416:G:H4'  | 1.80                     | 0.63              |
| 8:i:126:ARG:HA    | 8:i:129:GLU:HB2  | 1.81                     | 0.63              |
| 37:M:63:LYS:HB3   | 37:M:70:VAL:HG21 | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 46:V:18:LYS:HE2  | 52:3:255:G:H4'   | 1.80                     | 0.63              |
| 52:3:1033:G:H2'  | 52:3:1034:G:H5'' | 1.79                     | 0.63              |
| 53:1:1141:U:H4'  | 53:1:1142:A:O4'  | 1.98                     | 0.63              |
| 11:l:38:GLN:NE2  | 11:l:45:GLY:H    | 1.97                     | 0.63              |
| 14:o:30:ARG:HA   | 14:o:35:ILE:HG13 | 1.81                     | 0.63              |
| 16:q:56:PHE:HA   | 16:q:59:LEU:HD12 | 1.80                     | 0.63              |
| 20:u:4:ILE:HD12  | 20:u:4:ILE:N     | 2.14                     | 0.63              |
| 40:P:110:THR:HB  | 47:W:72:ARG:HH12 | 1.63                     | 0.63              |
| 1:b:101:ARG:HG2  | 1:b:103:ILE:HG23 | 1.81                     | 0.63              |
| 8:i:25:PRO:HB2   | 53:1:1095:A:N6   | 2.13                     | 0.63              |
| 38:N:51:LEU:HA   | 38:N:54:VAL:HG12 | 1.80                     | 0.63              |
| 1:b:93:VAL:HG21  | 1:b:103:ILE:HD11 | 1.81                     | 0.62              |
| 3:d:163:ASN:HB2  | 53:1:322:A:OP2   | 1.99                     | 0.62              |
| 17:r:78:ARG:HH12 | 53:1:990:A:H61   | 1.47                     | 0.62              |
| 33:I:44:LYS:HD2  | 33:I:45:PRO:HD2  | 1.81                     | 0.62              |
| 49:Y:23:ARG:NH2  | 52:3:1447:A:H61  | 1.97                     | 0.62              |
| 53:1:2508:G:H1   | 53:1:2580:U:H3   | 1.47                     | 0.62              |
| 6:g:40:THR:HB    | 6:g:43:ASN:HD22  | 1.64                     | 0.62              |
| 27:C:21:THR:HG22 | 53:1:2419:U:H5'' | 1.80                     | 0.62              |
| 54:2:72:G:H21    | 54:2:104:A:H62   | 1.45                     | 0.62              |
| 34:J:87:VAL:HA   | 34:J:91:SER:O    | 1.98                     | 0.62              |
| 49:Y:80:ALA:HA   | 49:Y:83:ASN:HD21 | 1.64                     | 0.62              |
| 53:1:1045:C:H5'  | 53:1:1046:A:H5'' | 1.80                     | 0.62              |
| 9:j:113:PRO:HG3  | 53:1:529:A:OP2   | 1.99                     | 0.62              |
| 6:g:46:PHE:HB3   | 6:g:50:ARG:HH21  | 1.64                     | 0.62              |
| 6:g:97:ARG:NH2   | 53:1:2220:U:H5'  | 2.13                     | 0.62              |
| 23:x:11:PRO:HG3  | 23:x:29:LEU:HD13 | 1.81                     | 0.62              |
| 25:z:41:PRO:HA   | 25:z:44:ARG:HB2  | 1.82                     | 0.62              |
| 31:G:20:ARG:HE   | 52:3:831:A:H4'   | 1.64                     | 0.62              |
| 51:a:55:SER:HA   | 51:a:58:ASN:ND2  | 2.15                     | 0.62              |
| 53:1:503:A:H4'   | 53:1:505:A:H5''  | 1.81                     | 0.62              |
| 5:f:157:LYS:HD2  | 53:1:2659:G:P    | 2.40                     | 0.62              |
| 12:m:45:GLN:NE2  | 53:1:2485:G:H5'' | 2.14                     | 0.62              |
| 17:r:79:ARG:NH2  | 53:1:572:A:H5'   | 2.15                     | 0.62              |
| 26:B:15:ARG:HH22 | 53:1:1264:A:H5'' | 1.64                     | 0.62              |
| 33:I:9:LYS:HD2   | 52:3:428:G:H5''  | 1.82                     | 0.62              |
| 37:M:12:ARG:HD2  | 37:M:26:MET:HE2  | 1.81                     | 0.62              |
| 41:Q:45:ASN:HB3  | 52:3:529:G:O6    | 1.99                     | 0.62              |
| 53:1:2818:U:H2'  | 53:1:2819:G:H8   | 1.64                     | 0.62              |
| 4:e:65:LEU:HD12  | 54:2:42:C:C4     | 2.35                     | 0.62              |
| 36:L:111:GLY:HA2 | 36:L:118:ARG:HD3 | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:N:10:ARG:HG3   | 38:N:105:ARG:HH21 | 1.63                     | 0.62              |
| 53:1:2688:G:H21   | 53:1:2721:A:H62   | 1.46                     | 0.62              |
| 36:L:87:PRO:HG3   | 36:L:148:LYS:HA   | 1.81                     | 0.62              |
| 8:i:117:THR:HG22  | 53:1:1058:U:H1'   | 1.81                     | 0.62              |
| 10:k:77:ILE:HG12  | 15:p:71:ARG:HG3   | 1.82                     | 0.62              |
| 8:i:21:PRO:HB2    | 8:i:22:PRO:HD3    | 1.80                     | 0.62              |
| 37:M:83:ARG:HH21  | 52:3:644:U:H5'    | 1.65                     | 0.62              |
| 23:x:7:THR:OG1    | 23:x:9:LYS:HE2    | 2.00                     | 0.61              |
| 23:x:36:ARG:HA    | 23:x:47:THR:HA    | 1.82                     | 0.61              |
| 38:N:115:VAL:HG23 | 39:O:62:ARG:HH11  | 1.64                     | 0.61              |
| 45:U:15:PRO:HD2   | 45:U:42:ILE:HD13  | 1.82                     | 0.61              |
| 49:Y:28:ARG:O     | 49:Y:31:ILE:HG22  | 2.00                     | 0.61              |
| 14:o:39:VAL:HB    | 14:o:49:VAL:HB    | 1.83                     | 0.61              |
| 35:K:79:ARG:HH12  | 52:3:672:U:H5'    | 1.65                     | 0.61              |
| 41:Q:98:ARG:HB2   | 41:Q:116:TYR:HA   | 1.82                     | 0.61              |
| 53:1:215:G:H4'    | 53:1:216:A:H4'    | 1.80                     | 0.61              |
| 53:1:821:A:H5''   | 53:1:822:G:H5'    | 1.83                     | 0.61              |
| 5:f:79:THR:HG23   | 5:f:80:GLU:HG3    | 1.81                     | 0.61              |
| 11:l:33:ARG:HH21  | 11:l:40:SER:HA    | 1.64                     | 0.61              |
| 16:q:18:LYS:HZ3   | 53:1:1219:U:P     | 2.22                     | 0.61              |
| 32:H:126:ARG:NH2  | 52:3:421:U:H3     | 1.98                     | 0.61              |
| 34:J:22:LYS:HG3   | 52:3:1081:A:H5'   | 1.81                     | 0.61              |
| 38:N:112:ARG:NH2  | 39:O:64:GLN:HE22  | 1.98                     | 0.61              |
| 53:1:1476:U:H3    | 53:1:1515:A:H62   | 1.45                     | 0.61              |
| 10:k:66:LYS:HB3   | 53:1:1665:A:H5''  | 1.83                     | 0.61              |
| 46:V:13:SER:HB2   | 46:V:21:VAL:CG1   | 2.31                     | 0.61              |
| 53:1:511:U:H2'    | 53:1:512:G:H5'    | 1.83                     | 0.61              |
| 1:b:145:MET:SD    | 1:b:181:ARG:NH2   | 2.73                     | 0.61              |
| 2:c:54:ALA:HA     | 2:c:76:GLY:HA2    | 1.80                     | 0.61              |
| 51:a:174:THR:HB   | 53:1:2124:G:C5'   | 2.30                     | 0.61              |
| 53:1:2298:A:H62   | 53:1:2318:G:H21   | 1.46                     | 0.61              |
| 57:7:71:G:H2'     | 57:7:72:C:H5''    | 1.82                     | 0.61              |
| 11:l:55:MET:HE3   | 53:1:2392:A:C2    | 2.36                     | 0.61              |
| 15:p:59:THR:HG22  | 15:p:72:VAL:HG12  | 1.82                     | 0.61              |
| 34:J:156:ARG:NH1  | 37:M:100:ILE:HG23 | 2.16                     | 0.61              |
| 53:1:226:A:H2'    | 53:1:227:A:O4'    | 2.00                     | 0.61              |
| 7:h:55:VAL:HA     | 53:1:1084:A:C4'   | 2.30                     | 0.61              |
| 32:H:102:ILE:HD12 | 32:H:102:ILE:N    | 2.15                     | 0.61              |
| 37:M:67:GLY:C     | 37:M:68:LYS:HD3   | 2.25                     | 0.61              |
| 46:V:58:VAL:CG2   | 46:V:74:LEU:HD11  | 2.29                     | 0.61              |
| 52:3:29:U:O2'     | 52:3:30:U:H5'     | 2.00                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:G:195:VAL:HB   | 31:G:198:VAL:HG12 | 1.81                     | 0.61              |
| 50:Z:23:GLU:O     | 50:Z:24:LYS:HB3   | 2.01                     | 0.61              |
| 53:1:2638:G:H1'   | 53:1:2778:A:H61   | 1.66                     | 0.61              |
| 57:7:44:G:H2'     | 57:7:45:U:H4'     | 1.83                     | 0.61              |
| 52:3:352:C:H4'    | 52:3:354:G:OP1    | 2.00                     | 0.61              |
| 52:3:428:G:H4'    | 52:3:429:U:O5'    | 2.00                     | 0.61              |
| 9:j:72:LYS:HB3    | 9:j:89:PHE:HB2    | 1.82                     | 0.61              |
| 19:t:40:LYS:HE2   | 19:t:60:THR:HG22  | 1.83                     | 0.61              |
| 21:v:53:LYS:HE3   | 21:v:55:GLU:HB2   | 1.83                     | 0.61              |
| 51:a:51:ASP:OD2   | 51:a:54:LYS:HG3   | 2.00                     | 0.61              |
| 53:1:2645:G:H4'   | 53:1:2732:G:H1'   | 1.83                     | 0.61              |
| 3:d:76:PRO:HA     | 3:d:82:GLY:HA2    | 1.83                     | 0.60              |
| 14:o:12:THR:HG21  | 53:1:2334:U:H5'   | 1.83                     | 0.60              |
| 55:6:54:U:H3      | 55:6:58:A:H62     | 1.49                     | 0.60              |
| 1:b:229:HIS:HE2   | 1:b:246:PRO:HG3   | 1.66                     | 0.60              |
| 26:B:30:ASP:HB3   | 26:B:34:GLY:H     | 1.66                     | 0.60              |
| 31:G:182:VAL:HG23 | 31:G:195:VAL:HG13 | 1.81                     | 0.60              |
| 37:M:46:GLU:HG2   | 37:M:61:THR:HB    | 1.83                     | 0.60              |
| 49:Y:6:ALA:HB2    | 52:3:107:G:H1     | 1.66                     | 0.60              |
| 1:b:43:ASN:ND2    | 1:b:45:ASN:HB2    | 2.14                     | 0.60              |
| 10:k:24:VAL:HA    | 10:k:39:ILE:HG22  | 1.83                     | 0.60              |
| 31:G:20:ARG:NE    | 52:3:831:A:H4'    | 2.16                     | 0.60              |
| 41:Q:48:LEU:HB2   | 52:3:520:A:OP1    | 2.00                     | 0.60              |
| 50:Z:66:ARG:HH21  | 52:3:1099:G:H4'   | 1.66                     | 0.60              |
| 52:3:1330:U:H2'   | 52:3:1331:G:O4'   | 2.01                     | 0.60              |
| 7:h:114:GLU:HA    | 7:h:123:ILE:HG12  | 1.83                     | 0.60              |
| 30:F:31:PRO:CB    | 53:1:2527:C:H5''  | 2.31                     | 0.60              |
| 34:J:20:VAL:HG11  | 52:3:1080:A:H4'   | 1.84                     | 0.60              |
| 39:O:10:LEU:HD23  | 39:O:10:LEU:H     | 1.66                     | 0.60              |
| 45:U:46:LYS:CE    | 52:3:617:G:H4'    | 2.31                     | 0.60              |
| 52:3:245:U:O2'    | 52:3:246:A:H5'    | 2.01                     | 0.60              |
| 52:3:1475:G:H4'   | 53:1:1689:A:H4'   | 1.83                     | 0.60              |
| 10:k:87:LEU:HA    | 10:k:94:PRO:HA    | 1.83                     | 0.60              |
| 14:o:51:ALA:HB3   | 14:o:78:VAL:HG12  | 1.83                     | 0.60              |
| 16:q:94:LEU:O     | 16:q:97:ILE:HG22  | 2.02                     | 0.60              |
| 53:1:1863:G:H4'   | 53:1:2411:A:H4'   | 1.81                     | 0.60              |
| 40:P:28:ASN:ND2   | 40:P:30:ILE:HB    | 2.16                     | 0.60              |
| 46:V:58:VAL:HG21  | 46:V:74:LEU:HD11  | 1.83                     | 0.60              |
| 55:6:16:C:H4'     | 55:6:60:U:H1'     | 1.84                     | 0.60              |
| 1:b:156:SER:OG    | 53:1:1819:A:H5''  | 2.02                     | 0.60              |
| 2:c:12:THR:HG22   | 2:c:13:ARG:H      | 1.66                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 50:Z:6:ARG:HG2   | 50:Z:8:ASN:H      | 1.67                     | 0.60              |
| 53:1:807:U:H2'   | 53:1:808:G:C8     | 2.37                     | 0.60              |
| 4:e:66:ILE:H     | 4:e:66:ILE:HD12   | 1.65                     | 0.60              |
| 20:u:32:LYS:NZ   | 53:1:478:A:H4'    | 2.16                     | 0.60              |
| 40:P:21:HIS:HA   | 40:P:84:MET:HB2   | 1.83                     | 0.60              |
| 38:N:86:LEU:HD23 | 38:N:97:LEU:HD22  | 1.84                     | 0.60              |
| 42:R:27:THR:HG21 | 52:3:1328:C:OP1   | 2.02                     | 0.60              |
| 54:2:3:C:C2'     | 54:2:4:C:H5''     | 2.32                     | 0.60              |
| 52:3:764:C:H2'   | 52:3:765:G:O4'    | 2.02                     | 0.60              |
| 52:3:946:A:H2'   | 52:3:947:G:C8     | 2.37                     | 0.60              |
| 1:b:120:ASP:HB2  | 6:g:91:PHE:HE1    | 1.67                     | 0.59              |
| 48:X:19:GLU:O    | 48:X:22:VAL:HG12  | 2.02                     | 0.59              |
| 32:H:69:THR:HG21 | 32:H:75:VAL:HG21  | 1.82                     | 0.59              |
| 43:S:12:ARG:HB3  | 43:S:59:GLN:HE22  | 1.67                     | 0.59              |
| 52:3:70:U:H5''   | 52:3:71:A:OP1     | 2.01                     | 0.59              |
| 53:1:2048:G:H3'  | 53:1:2049:G:H5''  | 1.83                     | 0.59              |
| 4:e:92:GLY:O     | 4:e:95:MET:HG2    | 2.02                     | 0.59              |
| 22:w:28:LEU:HD12 | 53:1:2354:C:OP1   | 2.02                     | 0.59              |
| 37:M:104:SER:HB2 | 37:M:125:ILE:HD11 | 1.84                     | 0.59              |
| 39:O:10:LEU:HD11 | 39:O:22:THR:HG22  | 1.84                     | 0.59              |
| 50:Z:34:ARG:HB3  | 50:Z:36:PHE:CE2   | 2.37                     | 0.59              |
| 50:Z:34:ARG:HB3  | 50:Z:36:PHE:CZ    | 2.37                     | 0.59              |
| 10:k:43:ILE:HG23 | 10:k:55:GLY:H     | 1.67                     | 0.59              |
| 14:o:29:HIS:CD2  | 54:2:7:G:H5''     | 2.38                     | 0.59              |
| 25:z:18:LYS:HE2  | 53:1:851:C:OP1    | 2.02                     | 0.59              |
| 33:I:120:LYS:HG2 | 33:I:130:ASN:HD21 | 1.68                     | 0.59              |
| 35:K:3:HIS:HB2   | 35:K:92:THR:HA    | 1.82                     | 0.59              |
| 53:1:1078:U:H5'' | 53:1:1079:C:H5''  | 1.85                     | 0.59              |
| 53:1:1912:A:H62  | 53:1:1917:U:H3    | 1.49                     | 0.59              |
| 44:T:5:GLU:HG2   | 44:T:6:ALA:N      | 2.18                     | 0.59              |
| 17:r:26:ASP:C    | 17:r:27:ILE:HD12  | 2.27                     | 0.59              |
| 18:s:49:LYS:O    | 18:s:52:GLU:HG3   | 2.02                     | 0.59              |
| 35:K:53:LYS:HG2  | 35:K:54:LEU:HD23  | 1.83                     | 0.59              |
| 53:1:2423:U:O2'  | 53:1:2425:A:H2'   | 2.02                     | 0.59              |
| 53:1:2480:C:H2'  | 53:1:2481:G:O4'   | 2.02                     | 0.59              |
| 6:g:68:ARG:HH21  | 6:g:72:ILE:HD11   | 1.67                     | 0.59              |
| 12:m:36:VAL:HG13 | 21:v:82:TYR:HB2   | 1.84                     | 0.59              |
| 42:R:108:ARG:NH1 | 52:3:1308:U:H5'   | 2.18                     | 0.59              |
| 49:Y:20:ASN:HD21 | 49:Y:65:LEU:HD13  | 1.68                     | 0.59              |
| 53:1:1026:G:H2'  | 53:1:1027:A:H8    | 1.68                     | 0.59              |
| 2:c:133:THR:HG21 | 53:1:1993:U:H4'   | 1.84                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:e:82:TYR:O     | 4:e:84:ILE:HG13   | 2.03                     | 0.59              |
| 5:f:27:GLY:HA3   | 5:f:78:VAL:HB     | 1.84                     | 0.59              |
| 38:N:8:THR:HG21  | 38:N:10:ARG:HH21  | 1.67                     | 0.59              |
| 53:1:2277:G:C2'  | 53:1:2278:A:H5''  | 2.32                     | 0.59              |
| 53:1:2834:G:H2'  | 53:1:2879:A:H61   | 1.67                     | 0.59              |
| 55:6:71:C:H2'    | 55:6:72:A:C8      | 2.38                     | 0.59              |
| 3:d:102:ARG:HG2  | 3:d:200:LEU:HG    | 1.85                     | 0.59              |
| 8:i:78:LEU:HD21  | 8:i:108:ILE:HG21  | 1.85                     | 0.59              |
| 12:m:122:ALA:HB1 | 53:1:2467:C:H1'   | 1.85                     | 0.59              |
| 35:K:29:ILE:HG13 | 35:K:34:GLY:HA3   | 1.84                     | 0.59              |
| 36:L:55:LYS:HB2  | 36:L:60:ALA:HB2   | 1.85                     | 0.59              |
| 42:R:113:LYS:CG  | 42:R:114:PRO:HD3  | 2.32                     | 0.59              |
| 47:W:32:ILE:HD11 | 47:W:67:LEU:HD22  | 1.85                     | 0.59              |
| 49:Y:19:HIS:O    | 49:Y:23:ARG:HD3   | 2.03                     | 0.59              |
| 55:5:13:C:C2'    | 55:5:14:A:H5''    | 2.30                     | 0.59              |
| 1:b:164:VAL:HG11 | 52:3:712:A:H5''   | 1.84                     | 0.58              |
| 3:d:77:ILE:HG13  | 3:d:78:TRP:HD1    | 1.68                     | 0.58              |
| 29:E:1:PRO:HG2   | 53:1:591:U:O2'    | 2.03                     | 0.58              |
| 35:K:7:VAL:HG22  | 35:K:61:LEU:HD12  | 1.85                     | 0.58              |
| 49:Y:67:HIS:O    | 49:Y:68:LYS:HG2   | 2.02                     | 0.58              |
| 6:g:25:TYR:HB2   | 53:1:2094:A:H5'   | 1.84                     | 0.58              |
| 31:G:103:TRP:HE1 | 31:G:107:ARG:HH21 | 1.51                     | 0.58              |
| 33:I:30:LYS:NZ   | 52:3:411:A:H2'    | 2.18                     | 0.58              |
| 33:I:95:GLY:O    | 33:I:136:VAL:HG22 | 2.02                     | 0.58              |
| 52:3:782:A:H62   | 52:3:800:G:H21    | 1.49                     | 0.58              |
| 4:e:39:VAL:HG13  | 4:e:40:GLY:H      | 1.67                     | 0.58              |
| 52:3:1506:U:O2'  | 52:3:1507:A:H5'   | 2.03                     | 0.58              |
| 53:1:1796:U:H2'  | 53:1:1797:G:H8    | 1.69                     | 0.58              |
| 58:5:101:FME:N   | 58:5:101:FME:SD   | 2.75                     | 0.58              |
| 17:r:42:ALA:HB2  | 17:r:46:GLU:HG2   | 1.84                     | 0.58              |
| 2:c:73:VAL:HG22  | 2:c:74:GLU:H      | 1.67                     | 0.58              |
| 4:e:39:VAL:HG22  | 4:e:41:GLU:H      | 1.68                     | 0.58              |
| 6:g:110:VAL:HG22 | 6:g:111:ALA:H     | 1.68                     | 0.58              |
| 41:Q:36:VAL:HG22 | 41:Q:52:CYS:SG    | 2.43                     | 0.58              |
| 43:S:84:ARG:HH12 | 52:3:1059:C:H4'   | 1.68                     | 0.58              |
| 44:T:23:SER:HB2  | 52:3:751:U:H4'    | 1.85                     | 0.58              |
| 48:X:10:ILE:HD13 | 48:X:40:PHE:CE2   | 2.38                     | 0.58              |
| 1:b:181:ARG:NH1  | 1:b:181:ARG:HB3   | 2.18                     | 0.58              |
| 2:c:5:VAL:H      | 2:c:32:ASN:HD21   | 1.52                     | 0.58              |
| 2:c:181:ASP:HB3  | 2:c:186:LEU:HB3   | 1.84                     | 0.58              |
| 2:c:192:ALA:HB1  | 53:1:2680:U:H1'   | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:C:28:THR:HG23  | 27:C:29:LYS:HG2   | 1.86                     | 0.58              |
| 38:N:23:GLY:H     | 38:N:60:LEU:HA    | 1.66                     | 0.58              |
| 41:Q:81:ILE:HG13  | 41:Q:95:HIS:O     | 2.04                     | 0.58              |
| 44:T:52:ARG:CZ    | 53:1:715:A:H61    | 2.17                     | 0.58              |
| 53:1:1932:A:H62   | 53:1:1968:G:H21   | 1.51                     | 0.58              |
| 8:i:12:VAL:O      | 8:i:13:ALA:C      | 2.46                     | 0.58              |
| 45:U:67:ILE:HD11  | 45:U:71:VAL:HG12  | 1.86                     | 0.58              |
| 47:W:40:PRO:HG2   | 47:W:43:ILE:HD13  | 1.86                     | 0.58              |
| 52:3:225:C:H2'    | 52:3:226:G:H5''   | 1.86                     | 0.58              |
| 53:1:1367:A:H2'   | 53:1:1368:G:H5'   | 1.84                     | 0.58              |
| 1:b:204:LEU:HD12  | 53:1:1791:A:H5''  | 1.85                     | 0.58              |
| 8:i:74:PRO:HB2    | 8:i:77:VAL:HG22   | 1.85                     | 0.58              |
| 11:l:57:LEU:HD11  | 29:E:56:LEU:HD13  | 1.86                     | 0.58              |
| 32:H:56:ILE:HG23  | 32:H:63:ILE:HD11  | 1.86                     | 0.58              |
| 53:1:1373:A:H4'   | 53:1:2212:A:H1'   | 1.84                     | 0.58              |
| 53:1:2156:G:H2'   | 53:1:2157:G:H5'   | 1.85                     | 0.58              |
| 54:2:78:A:H62     | 54:2:98:G:H21     | 1.51                     | 0.58              |
| 12:m:13:HIS:HE1   | 53:1:2265:U:H4'   | 1.69                     | 0.58              |
| 19:t:73:ARG:HH22  | 53:1:456:C:H2'    | 1.68                     | 0.58              |
| 52:3:77:A:H2'     | 52:3:78:A:H8      | 1.68                     | 0.58              |
| 36:L:36:SER:O     | 36:L:39:GLU:HG2   | 2.03                     | 0.58              |
| 4:e:111:ARG:NH1   | 4:e:132:ARG:HD2   | 2.18                     | 0.57              |
| 26:B:8:THR:HG23   | 26:B:11:LYS:H     | 1.70                     | 0.57              |
| 28:D:3:ARG:HG2    | 53:1:1613:G:H4'   | 1.85                     | 0.57              |
| 28:D:42:LEU:HD12  | 28:D:42:LEU:H     | 1.69                     | 0.57              |
| 33:I:30:LYS:HZ3   | 52:3:411:A:H2'    | 1.69                     | 0.57              |
| 43:S:20:PHE:O     | 43:S:21:ALA:HB3   | 2.04                     | 0.57              |
| 6:g:63:ALA:HA     | 6:g:66:ASN:HD22   | 1.69                     | 0.57              |
| 12:m:60:GLN:HE21  | 12:m:108:VAL:HG12 | 1.68                     | 0.57              |
| 20:u:26:ASN:HD21  | 20:u:34:ILE:HD12  | 1.68                     | 0.57              |
| 32:H:124:GLU:HG3  | 32:H:125:ARG:HH11 | 1.68                     | 0.57              |
| 7:h:2:ALA:O       | 53:1:1043:C:H5''  | 2.03                     | 0.57              |
| 10:k:35:VAL:HG13  | 10:k:36:GLY:H     | 1.69                     | 0.57              |
| 12:m:26:VAL:HB    | 12:m:133:LYS:HA   | 1.85                     | 0.57              |
| 18:s:33:LEU:HD11  | 18:s:55:ILE:HD11  | 1.87                     | 0.57              |
| 18:s:52:GLU:OE1   | 53:1:488:G:H5'    | 2.04                     | 0.57              |
| 34:J:163:ILE:HD12 | 34:J:163:ILE:H    | 1.69                     | 0.57              |
| 43:S:44:VAL:HG13  | 43:S:45:LEU:HD22  | 1.86                     | 0.57              |
| 53:1:2432:A:H1'   | 55:6:75:C:C4'     | 2.33                     | 0.57              |
| 4:e:46:LYS:HD2    | 4:e:47:LYS:HG3    | 1.87                     | 0.57              |
| 9:j:64:VAL:HB     | 9:j:68:LYS:HE3    | 1.87                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 14:o:33:ARG:HB2   | 54:2:52:A:N6     | 2.20                     | 0.57              |
| 20:u:14:THR:OG1   | 53:1:310:A:H5''  | 2.04                     | 0.57              |
| 50:Z:9:GLU:HB3    | 50:Z:10:PRO:CD   | 2.34                     | 0.57              |
| 52:3:235:C:H2'    | 52:3:236:A:C8    | 2.40                     | 0.57              |
| 52:3:1432:G:H1'   | 52:3:1468:A:N6   | 2.19                     | 0.57              |
| 1:b:106:PRO:HG2   | 1:b:109:LEU:HB2  | 1.87                     | 0.57              |
| 20:u:42:LYS:CE    | 53:1:499:U:H5''  | 2.35                     | 0.57              |
| 8:i:58:ILE:H      | 8:i:58:ILE:HD12  | 1.70                     | 0.57              |
| 34:J:133:ILE:HG23 | 34:J:134:ASN:OD1 | 2.04                     | 0.57              |
| 37:M:80:PRO:HG2   | 52:3:878:A:H5'   | 1.86                     | 0.57              |
| 53:1:2286:G:H4'   | 53:1:2287:A:O5'  | 2.05                     | 0.57              |
| 2:c:187:LEU:HD23  | 2:c:187:LEU:O    | 2.05                     | 0.57              |
| 15:p:102:ARG:NH2  | 53:1:1754:A:O3'  | 2.36                     | 0.57              |
| 18:s:79:GLY:C     | 53:1:25:U:H4'    | 2.30                     | 0.57              |
| 24:y:16:THR:HA    | 24:y:19:LEU:HD12 | 1.86                     | 0.57              |
| 28:D:9:VAL:HG22   | 53:1:1309:G:OP1  | 2.05                     | 0.57              |
| 33:I:71:PHE:HA    | 33:I:74:TYR:HB2  | 1.87                     | 0.57              |
| 34:J:73:VAL:HG11  | 34:J:143:LEU:HB3 | 1.86                     | 0.57              |
| 52:3:1308:U:H2'   | 52:3:1309:G:C8   | 2.40                     | 0.57              |
| 53:1:818:G:H21    | 53:1:1189:A:H62  | 1.53                     | 0.57              |
| 1:b:129:LEU:N     | 1:b:129:LEU:HD23 | 2.20                     | 0.57              |
| 3:d:117:ARG:NH1   | 11:l:2:ARG:HE    | 2.02                     | 0.57              |
| 15:p:112:ARG:O    | 15:p:114:ASN:N   | 2.38                     | 0.57              |
| 53:1:489:G:H22    | 53:1:1320:C:H3'  | 1.70                     | 0.57              |
| 57:7:7:A:H3'      | 57:7:8:U:C5'     | 2.35                     | 0.57              |
| 57:7:44:G:H2'     | 57:7:45:U:C4'    | 2.35                     | 0.57              |
| 3:d:69:ARG:HH12   | 53:1:2060:A:N6   | 2.00                     | 0.57              |
| 21:v:11:GLU:HG3   | 21:v:16:ALA:HB1  | 1.87                     | 0.57              |
| 36:L:145:GLU:HA   | 36:L:148:LYS:HB2 | 1.87                     | 0.57              |
| 40:P:83:VAL:HB    | 40:P:109:ILE:HA  | 1.87                     | 0.57              |
| 43:S:26:LEU:HA    | 43:S:30:ILE:HD13 | 1.87                     | 0.57              |
| 53:1:1186:G:H2'   | 53:1:1187:G:O4'  | 2.05                     | 0.57              |
| 11:l:70:LYS:HA    | 11:l:73:ILE:HG12 | 1.87                     | 0.57              |
| 20:u:3:LYS:HD3    | 20:u:82:VAL:HB   | 1.87                     | 0.57              |
| 53:1:1509:A:H2'   | 53:1:1510:G:C8   | 2.40                     | 0.57              |
| 1:b:260:LYS:HA    | 1:b:263:ASP:OD2  | 2.05                     | 0.56              |
| 4:e:140:ILE:HG13  | 4:e:142:TYR:H    | 1.70                     | 0.56              |
| 5:f:8:VAL:HB      | 5:f:49:LEU:HB2   | 1.86                     | 0.56              |
| 5:f:88:LEU:HD21   | 5:f:95:ALA:HB2   | 1.86                     | 0.56              |
| 9:j:13:ARG:CD     | 9:j:121:LYS:HE2  | 2.35                     | 0.56              |
| 34:J:28:ARG:HH12  | 52:3:15:G:H4'    | 1.69                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 44:T:64:LYS:O    | 44:T:67:ASP:OD1   | 2.23                     | 0.56              |
| 53:1:2417:C:H2'  | 53:1:2418:A:C8    | 2.40                     | 0.56              |
| 11:l:82:LEU:HD12 | 11:l:120:VAL:HG11 | 1.87                     | 0.56              |
| 37:M:54:THR:C    | 37:M:56:PRO:HD3   | 2.30                     | 0.56              |
| 51:a:7:ARG:HH22  | 51:a:35:THR:HB    | 1.69                     | 0.56              |
| 52:3:1502:A:H5'  | 52:3:1504:G:N7    | 2.18                     | 0.56              |
| 53:1:479:A:H4'   | 53:1:480:A:H5'    | 1.87                     | 0.56              |
| 4:e:107:VAL:CG1  | 4:e:108:PRO:HD3   | 2.34                     | 0.56              |
| 8:i:71:LYS:HD3   | 8:i:72:THR:N      | 2.19                     | 0.56              |
| 19:t:10:VAL:HG11 | 19:t:42:GLU:OE1   | 2.05                     | 0.56              |
| 38:N:126:PHE:HZ  | 52:3:967:C:H4'    | 1.69                     | 0.56              |
| 40:P:86:LYS:HG3  | 40:P:114:PRO:HD3  | 1.86                     | 0.56              |
| 41:Q:117:GLY:HA2 | 52:3:35:G:O2'     | 2.04                     | 0.56              |
| 42:R:25:GLY:N    | 52:3:1329:A:H5''  | 2.20                     | 0.56              |
| 47:W:35:SER:HA   | 47:W:71:ASP:HB3   | 1.87                     | 0.56              |
| 52:3:150:U:H3    | 52:3:171:A:H62    | 1.54                     | 0.56              |
| 52:3:1202:U:H2'  | 52:3:1203:C:H5'   | 1.87                     | 0.56              |
| 53:1:615:U:H5''  | 53:1:616:A:OP2    | 2.04                     | 0.56              |
| 53:1:1837:C:H2'  | 53:1:1899:A:H61   | 1.70                     | 0.56              |
| 53:1:2048:G:H2'  | 53:1:2049:G:H5''  | 1.87                     | 0.56              |
| 20:u:71:ILE:H    | 20:u:71:ILE:HD12  | 1.70                     | 0.56              |
| 48:X:35:ARG:NH2  | 48:X:74:ALA:HB3   | 2.21                     | 0.56              |
| 40:P:44:ALA:HB3  | 40:P:69:CYS:HB2   | 1.88                     | 0.56              |
| 42:R:16:ILE:HD11 | 52:3:1302:C:P     | 2.45                     | 0.56              |
| 48:X:10:ILE:HD13 | 48:X:40:PHE:HE2   | 1.70                     | 0.56              |
| 53:1:995:C:H6    | 53:1:995:C:H5'    | 1.71                     | 0.56              |
| 53:1:2457:U:H3   | 53:1:2494:G:H1    | 1.53                     | 0.56              |
| 54:2:55:U:H2'    | 54:2:56:G:C8      | 2.41                     | 0.56              |
| 3:d:127:GLU:HG2  | 3:d:128:ALA:H     | 1.69                     | 0.56              |
| 53:1:1874:C:H2'  | 53:1:1875:G:O4'   | 2.06                     | 0.56              |
| 1:b:55:GLY:H     | 53:1:692:C:P      | 2.29                     | 0.56              |
| 6:g:97:ARG:HH12  | 53:1:2220:U:H5''  | 1.70                     | 0.56              |
| 7:h:61:ARG:HB3   | 53:1:1046:A:H4'   | 1.88                     | 0.56              |
| 22:w:64:LYS:HG2  | 22:w:66:GLU:OE2   | 2.05                     | 0.56              |
| 23:x:29:LEU:HD12 | 23:x:30:PRO:HD2   | 1.86                     | 0.56              |
| 31:G:24:PRO:HB3  | 52:3:828:U:H2'    | 1.88                     | 0.56              |
| 34:J:61:LYS:HE3  | 52:3:1073:U:OP2   | 2.05                     | 0.56              |
| 45:U:5:ARG:HA    | 45:U:71:VAL:HG21  | 1.87                     | 0.56              |
| 53:1:668:A:H2'   | 53:1:670:A:H62    | 1.71                     | 0.56              |
| 39:O:53:ILE:HG12 | 39:O:61:ALA:O     | 2.06                     | 0.56              |
| 43:S:62:ARG:HD3  | 43:S:67:GLY:O     | 2.06                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 44:T:65:LEU:HD23  | 52:3:754:C:O2'   | 2.05                     | 0.56              |
| 53:1:118:A:OP2    | 53:1:119:A:H2'   | 2.06                     | 0.56              |
| 7:h:23:LEU:HG     | 7:h:118:ILE:HD12 | 1.88                     | 0.56              |
| 14:o:11:ALA:HB2   | 14:o:96:GLY:N    | 2.20                     | 0.56              |
| 18:s:6:LYS:HG3    | 53:1:494:G:H4'   | 1.87                     | 0.56              |
| 19:t:88:LYS:HG2   | 19:t:89:GLU:H    | 1.70                     | 0.56              |
| 30:F:36:ARG:NH2   | 53:1:2742:G:H5'  | 2.20                     | 0.56              |
| 51:a:37:LYS:HG3   | 53:1:2128:G:OP1  | 2.06                     | 0.56              |
| 52:3:70:U:H2'     | 52:3:94:G:O6     | 2.06                     | 0.56              |
| 53:1:1111:A:O2'   | 53:1:1112:G:H4'  | 2.05                     | 0.56              |
| 1:b:208:GLY:C     | 1:b:210:ALA:H    | 2.13                     | 0.56              |
| 16:q:8:ILE:HG23   | 16:q:9:ALA:H     | 1.71                     | 0.56              |
| 33:I:125:ASN:HD21 | 33:I:140:ASP:HB3 | 1.71                     | 0.56              |
| 49:Y:22:SER:HA    | 52:3:1458:G:O3'  | 2.05                     | 0.56              |
| 53:1:307:G:H21    | 53:1:330:A:H61   | 1.54                     | 0.56              |
| 53:1:441:U:O2'    | 53:1:442:G:H5'   | 2.06                     | 0.56              |
| 53:1:1138:G:H2'   | 53:1:1139:G:O4'  | 2.05                     | 0.56              |
| 53:1:2328:A:H2'   | 53:1:2329:U:C6   | 2.41                     | 0.56              |
| 17:r:78:ARG:HB3   | 17:r:83:TYR:HB3  | 1.87                     | 0.55              |
| 28:D:11:LYS:HE3   | 53:1:686:U:C5'   | 2.36                     | 0.55              |
| 50:Z:18:PHE:HA    | 50:Z:21:SER:HB3  | 1.88                     | 0.55              |
| 52:3:1160:G:H1    | 52:3:1176:A:H61  | 1.54                     | 0.55              |
| 52:3:1271:A:H5'   | 52:3:1314:C:H5'  | 1.86                     | 0.55              |
| 1:b:180:MET:HB2   | 1:b:268:ARG:HB2  | 1.89                     | 0.55              |
| 12:m:58:LYS:O     | 12:m:60:GLN:N    | 2.38                     | 0.55              |
| 15:p:77:SER:O     | 15:p:80:VAL:HG12 | 2.06                     | 0.55              |
| 19:t:33:LYS:HE3   | 19:t:80:TRP:CZ3  | 2.41                     | 0.55              |
| 38:N:34:LEU:HD23  | 38:N:34:LEU:H    | 1.70                     | 0.55              |
| 39:O:80:THR:HG22  | 39:O:82:LYS:H    | 1.71                     | 0.55              |
| 41:Q:73:LEU:HD21  | 41:Q:79:ILE:HD13 | 1.89                     | 0.55              |
| 48:X:30:LEU:HD13  | 48:X:48:ILE:HG22 | 1.89                     | 0.55              |
| 49:Y:61:ALA:HA    | 49:Y:66:ILE:HB   | 1.88                     | 0.55              |
| 53:1:2432:A:H1'   | 55:6:75:C:H4'    | 1.88                     | 0.55              |
| 55:5:6:G:O2'      | 55:5:7:G:H5'     | 2.07                     | 0.55              |
| 3:d:68:ALA:HA     | 53:1:1255:U:C6   | 2.42                     | 0.55              |
| 3:d:101:TYR:HE1   | 3:d:177:PRO:HG3  | 1.71                     | 0.55              |
| 20:u:32:LYS:HZ3   | 53:1:478:A:H4'   | 1.71                     | 0.55              |
| 21:v:78:GLN:HE22  | 54:2:76:G:H21    | 1.54                     | 0.55              |
| 35:K:67:PRO:HG2   | 35:K:70:VAL:HG12 | 1.89                     | 0.55              |
| 36:L:85:GLN:HB2   | 36:L:147:ASN:ND2 | 2.21                     | 0.55              |
| 50:Z:23:GLU:C     | 50:Z:25:ALA:H    | 2.15                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 53:1:1680:U:H2'   | 53:1:1681:G:H5'  | 1.88                     | 0.55              |
| 53:1:2287:A:O2'   | 53:1:2288:A:H2'  | 2.05                     | 0.55              |
| 53:1:2747:G:H21   | 53:1:2757:A:H62  | 1.52                     | 0.55              |
| 15:p:61:ARG:HE    | 15:p:99:LEU:HG   | 1.71                     | 0.55              |
| 31:G:100:LEU:HD12 | 31:G:174:GLU:HB3 | 1.87                     | 0.55              |
| 32:H:1:GLY:HA3    | 52:3:1060:U:H5   | 1.71                     | 0.55              |
| 38:N:16:ALA:HB2   | 38:N:77:ALA:HB1  | 1.88                     | 0.55              |
| 15:p:46:VAL:HA    | 15:p:60:VAL:HA   | 1.88                     | 0.55              |
| 6:g:69:ALA:HA     | 6:g:72:ILE:HG13  | 1.88                     | 0.55              |
| 8:i:72:THR:HG23   | 8:i:73:PRO:HD2   | 1.88                     | 0.55              |
| 52:3:184:G:H4'    | 52:3:224:U:H4'   | 1.87                     | 0.55              |
| 53:1:346:A:H2'    | 53:1:346:A:N3    | 2.21                     | 0.55              |
| 53:1:2533:U:H2'   | 53:1:2534:A:O4'  | 2.07                     | 0.55              |
| 2:c:53:GLY:HA3    | 2:c:77:ARG:HH21  | 1.71                     | 0.55              |
| 4:e:34:THR:HA     | 4:e:89:THR:HA    | 1.87                     | 0.55              |
| 32:H:31:ASN:HD22  | 32:H:58:ARG:HH11 | 1.54                     | 0.55              |
| 35:K:79:ARG:HH12  | 52:3:672:U:C5'   | 2.19                     | 0.55              |
| 45:U:14:ARG:HH12  | 52:3:618:C:H1'   | 1.71                     | 0.55              |
| 35:K:9:MET:HB3    | 35:K:57:ALA:HB1  | 1.89                     | 0.55              |
| 35:K:79:ARG:NH1   | 52:3:672:U:H5'   | 2.21                     | 0.55              |
| 39:O:52:LEU:HB2   | 43:S:80:ARG:HD2  | 1.87                     | 0.55              |
| 7:h:94:ARG:HE     | 7:h:131:THR:HG22 | 1.72                     | 0.55              |
| 17:r:35:PHE:HB2   | 17:r:59:ILE:HB   | 1.89                     | 0.55              |
| 33:I:119:HIS:CE1  | 52:3:438:U:H4'   | 2.42                     | 0.55              |
| 46:V:48:GLU:O     | 46:V:50:ASN:N    | 2.39                     | 0.55              |
| 53:1:582:A:H2'    | 53:1:583:G:H8    | 1.72                     | 0.55              |
| 53:1:940:G:H3'    | 53:1:941:A:H5''  | 1.89                     | 0.55              |
| 53:1:1019:U:H2'   | 53:1:1020:A:H8   | 1.71                     | 0.55              |
| 4:e:28:PRO:HB2    | 4:e:168:LEU:HD21 | 1.87                     | 0.55              |
| 8:i:12:VAL:HG12   | 8:i:13:ALA:H     | 1.72                     | 0.55              |
| 46:V:37:ILE:HB    | 46:V:39:ARG:HE   | 1.71                     | 0.55              |
| 53:1:1614:A:H2'   | 53:1:1615:C:H5'  | 1.89                     | 0.55              |
| 53:1:2277:G:C3'   | 53:1:2278:A:H5'' | 2.36                     | 0.55              |
| 1:b:52:HIS:NE2    | 53:1:1824:G:OP2  | 2.40                     | 0.54              |
| 10:k:109:SER:O    | 10:k:110:GLU:HG2 | 2.07                     | 0.54              |
| 18:s:42:LYS:CB    | 53:1:2010:G:H5'' | 2.37                     | 0.54              |
| 32:H:172:VAL:HG23 | 52:3:1107:C:H5'' | 1.89                     | 0.54              |
| 34:J:133:ILE:HG23 | 34:J:134:ASN:N   | 2.22                     | 0.54              |
| 36:L:24:LYS:O     | 36:L:28:ILE:HG13 | 2.07                     | 0.54              |
| 53:1:2623:G:H2'   | 53:1:2624:G:H8   | 1.72                     | 0.54              |
| 2:c:129:THR:OG1   | 2:c:140:HIS:O    | 2.23                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 28:D:45:SER:OG   | 28:D:46:LYS:N     | 2.40                     | 0.54              |
| 37:M:44:PHE:CZ   | 37:M:128:VAL:HG11 | 2.43                     | 0.54              |
| 40:P:15:VAL:HG22 | 40:P:16:SER:N     | 2.20                     | 0.54              |
| 52:3:715:A:H2'   | 52:3:716:A:C8     | 2.43                     | 0.54              |
| 53:1:399:U:OP1   | 53:1:2090:A:H5''  | 2.08                     | 0.54              |
| 53:1:1344:U:H3'  | 53:1:1345:C:H5'   | 1.88                     | 0.54              |
| 1:b:237:ARG:HD2  | 53:1:2590:A:H5''  | 1.88                     | 0.54              |
| 2:c:5:VAL:H      | 2:c:32:ASN:ND2    | 2.04                     | 0.54              |
| 2:c:78:GLY:C     | 2:c:79:LEU:HD12   | 2.32                     | 0.54              |
| 3:d:1:MET:HE3    | 3:d:2:GLU:H       | 1.72                     | 0.54              |
| 12:m:74:THR:HA   | 12:m:89:VAL:HA    | 1.90                     | 0.54              |
| 16:q:47:ARG:O    | 16:q:51:GLN:HG2   | 2.07                     | 0.54              |
| 18:s:35:ILE:O    | 18:s:39:THR:HG23  | 2.06                     | 0.54              |
| 22:w:63:VAL:HG12 | 22:w:78:ILE:HG12  | 1.90                     | 0.54              |
| 52:3:1005:A:H2'  | 52:3:1006:G:O4'   | 2.08                     | 0.54              |
| 53:1:324:A:H62   | 53:1:338:G:H21    | 1.55                     | 0.54              |
| 53:1:669:G:H2'   | 53:1:669:G:N3     | 2.23                     | 0.54              |
| 53:1:1597:A:H5'' | 53:1:1598:A:H5'   | 1.88                     | 0.54              |
| 53:1:2818:U:H2'  | 53:1:2819:G:C8    | 2.43                     | 0.54              |
| 1:b:254:LYS:O    | 53:1:1797:G:H4'   | 2.08                     | 0.54              |
| 3:d:40:ARG:HD2   | 53:1:443:A:C5     | 2.41                     | 0.54              |
| 10:k:48:PRO:HA   | 52:3:1422:G:OP1   | 2.08                     | 0.54              |
| 13:n:48:VAL:O    | 13:n:52:ILE:HD12  | 2.07                     | 0.54              |
| 17:r:1:MET:N     | 17:r:1:MET:SD     | 2.79                     | 0.54              |
| 17:r:83:TYR:CE1  | 53:1:1187:G:H5''  | 2.43                     | 0.54              |
| 23:x:10:ARG:NH2  | 53:1:187:G:H4'    | 2.23                     | 0.54              |
| 23:x:17:ARG:HD2  | 23:x:21:LEU:HD22  | 1.89                     | 0.54              |
| 34:J:54:GLU:HB3  | 34:J:57:ALA:HB3   | 1.90                     | 0.54              |
| 49:Y:32:LYS:HA   | 49:Y:35:TYR:HB2   | 1.90                     | 0.54              |
| 52:3:501:C:H2'   | 52:3:502:A:C8     | 2.42                     | 0.54              |
| 53:1:821:A:H5''  | 53:1:822:G:H5''   | 1.90                     | 0.54              |
| 53:1:1547:C:H2'  | 53:1:1548:A:H8    | 1.73                     | 0.54              |
| 53:1:2636:C:H2'  | 53:1:2637:U:C6    | 2.42                     | 0.54              |
| 1:b:256:THR:OG1  | 53:1:1798:U:H5'   | 2.08                     | 0.54              |
| 5:f:92:GLY:H     | 5:f:94:ARG:NH1    | 2.06                     | 0.54              |
| 19:t:51:PHE:O    | 19:t:52:GLU:HG2   | 2.08                     | 0.54              |
| 23:x:29:LEU:HG   | 53:1:2230:G:H4'   | 1.90                     | 0.54              |
| 39:O:22:THR:O    | 39:O:26:VAL:HG23  | 2.08                     | 0.54              |
| 52:3:572:A:H5''  | 52:3:917:G:H4'    | 1.89                     | 0.54              |
| 53:1:655:A:H4'   | 53:1:656:G:H5'    | 1.89                     | 0.54              |
| 53:1:2417:C:H2'  | 53:1:2418:A:H8    | 1.72                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:b:216:ARG:HH21 | 53:1:780:G:H5''   | 1.73                     | 0.54              |
| 1:b:220:ARG:HD2  | 53:1:1827:U:OP2   | 2.08                     | 0.54              |
| 2:c:56:LYS:NZ    | 53:1:2830:C:H5''  | 2.22                     | 0.54              |
| 2:c:148:GLN:HG3  | 53:1:2574:G:N3    | 2.23                     | 0.54              |
| 5:f:86:LEU:HB2   | 5:f:130:ILE:HG23  | 1.89                     | 0.54              |
| 13:n:66:ALA:HB2  | 13:n:80:PHE:HE2   | 1.73                     | 0.54              |
| 36:L:27:ASN:HB3  | 52:3:1374:A:O2'   | 2.07                     | 0.54              |
| 39:O:30:LYS:CE   | 39:O:36:VAL:HG22  | 2.37                     | 0.54              |
| 52:3:265:G:H2'   | 52:3:267:C:H5     | 1.73                     | 0.54              |
| 53:1:2831:G:H1'  | 53:1:2883:A:H2'   | 1.88                     | 0.54              |
| 1:b:162:GLN:HB3  | 1:b:174:ARG:HB3   | 1.90                     | 0.54              |
| 14:o:40:ILE:HG12 | 14:o:47:VAL:HG12  | 1.88                     | 0.54              |
| 15:p:3:ILE:H     | 15:p:3:ILE:HD12   | 1.73                     | 0.54              |
| 19:t:57:VAL:HG22 | 19:t:86:THR:OG1   | 2.06                     | 0.54              |
| 32:H:67:ILE:HD12 | 32:H:67:ILE:N     | 2.23                     | 0.54              |
| 33:I:28:ASP:O    | 33:I:29:THR:HG22  | 2.08                     | 0.54              |
| 37:M:42:GLU:OE1  | 37:M:100:ILE:HD13 | 2.08                     | 0.54              |
| 38:N:46:VAL:HG21 | 38:N:75:ALA:HB1   | 1.89                     | 0.54              |
| 40:P:35:ASP:OD1  | 40:P:39:ASN:N     | 2.39                     | 0.54              |
| 42:R:112:ARG:HD3 | 52:3:1229:A:P     | 2.48                     | 0.54              |
| 46:V:46:HIS:H    | 46:V:73:THR:HA    | 1.73                     | 0.54              |
| 53:1:554:U:H2'   | 53:1:555:G:O4'    | 2.08                     | 0.54              |
| 53:1:955:U:H3    | 53:1:962:G:H1     | 1.54                     | 0.54              |
| 23:x:13:THR:HG21 | 53:1:188:G:H5'    | 1.90                     | 0.54              |
| 52:3:361:G:H2'   | 52:3:362:G:O4'    | 2.08                     | 0.54              |
| 53:1:742:A:H2'   | 53:1:743:A:C8     | 2.42                     | 0.54              |
| 53:1:828:U:H4'   | 53:1:831:G:N1     | 2.23                     | 0.54              |
| 1:b:270:ARG:NH1  | 1:b:270:ARG:HB3   | 2.23                     | 0.54              |
| 5:f:71:LEU:O     | 5:f:75:VAL:HG23   | 2.08                     | 0.54              |
| 7:h:48:ALA:HB3   | 7:h:51:TYR:CE1    | 2.42                     | 0.54              |
| 7:h:61:ARG:O     | 53:1:1046:A:H4'   | 2.08                     | 0.54              |
| 7:h:94:ARG:HA    | 7:h:129:LEU:HD13  | 1.89                     | 0.54              |
| 36:L:22:LEU:O    | 36:L:26:VAL:HG23  | 2.08                     | 0.54              |
| 41:Q:85:ARG:HA   | 41:Q:93:ARG:HA    | 1.90                     | 0.54              |
| 48:X:18:VAL:HG11 | 48:X:43:MET:HG2   | 1.90                     | 0.54              |
| 3:d:162:ARG:NE   | 53:1:322:A:OP1    | 2.37                     | 0.54              |
| 51:a:201:PRO:HB2 | 51:a:204:ALA:HB2  | 1.90                     | 0.54              |
| 53:1:940:G:C3'   | 53:1:941:A:H5''   | 2.38                     | 0.54              |
| 53:1:2553:G:C3'  | 53:1:2554:U:H5''  | 2.38                     | 0.54              |
| 1:b:100:ARG:HH22 | 53:1:1500:G:H4'   | 1.74                     | 0.53              |
| 11:l:38:GLN:HB2  | 53:1:831:G:O2'    | 2.08                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:c:190:LYS:HG2  | 2:c:191:GLY:N     | 2.23                     | 0.53              |
| 7:h:21:GLY:HA3   | 7:h:86:MET:HG3    | 1.91                     | 0.53              |
| 7:h:29:ASP:HB3   | 7:h:32:GLY:HA3    | 1.90                     | 0.53              |
| 20:u:27:VAL:HA   | 20:u:33:VAL:HA    | 1.91                     | 0.53              |
| 35:K:10:VAL:HG22 | 35:K:11:HIS:H     | 1.73                     | 0.53              |
| 41:Q:4:ASN:HB3   | 52:3:880:C:OP2    | 2.09                     | 0.53              |
| 41:Q:77:SER:HB2  | 41:Q:102:ASP:HB3  | 1.90                     | 0.53              |
| 52:3:521:G:H21   | 52:3:536:C:H5'    | 1.73                     | 0.53              |
| 52:3:948:C:H2'   | 52:3:949:A:H8     | 1.73                     | 0.53              |
| 53:1:310:A:H2'   | 53:1:311:A:H5''   | 1.90                     | 0.53              |
| 53:1:1020:A:C1'  | 53:1:1021:A:OP2   | 2.54                     | 0.53              |
| 53:1:2128:G:H1'  | 53:1:2173:A:N3    | 2.23                     | 0.53              |
| 6:g:110:VAL:HG22 | 6:g:111:ALA:N     | 2.22                     | 0.53              |
| 15:p:51:ASN:ND2  | 53:1:2845:U:OP1   | 2.40                     | 0.53              |
| 34:J:93:VAL:HA   | 34:J:126:ALA:HA   | 1.90                     | 0.53              |
| 40:P:125:LYS:HD2 | 52:3:797:C:P      | 2.48                     | 0.53              |
| 1:b:174:ARG:HE   | 1:b:180:MET:HE1   | 1.72                     | 0.53              |
| 2:c:133:THR:CG2  | 53:1:1993:U:H4'   | 2.38                     | 0.53              |
| 5:f:32:LEU:HD22  | 5:f:74:MET:HE3    | 1.90                     | 0.53              |
| 10:k:63:VAL:HG13 | 10:k:64:ARG:N     | 2.22                     | 0.53              |
| 15:p:51:ASN:O    | 53:1:2845:U:H5''  | 2.08                     | 0.53              |
| 18:s:4:ILE:HG22  | 18:s:106:VAL:HG13 | 1.91                     | 0.53              |
| 19:t:53:VAL:HG11 | 19:t:87:LEU:HD13  | 1.89                     | 0.53              |
| 19:t:61:LEU:HB3  | 53:1:1341:G:H5'   | 1.91                     | 0.53              |
| 27:C:21:THR:HG23 | 29:E:33:THR:HB    | 1.91                     | 0.53              |
| 52:3:211:G:H2'   | 52:3:212:G:H5'    | 1.90                     | 0.53              |
| 53:1:161:A:H3'   | 53:1:162:U:H5''   | 1.90                     | 0.53              |
| 53:1:367:G:H2'   | 53:1:368:A:O4'    | 2.08                     | 0.53              |
| 8:i:33:ASN:HD22  | 8:i:36:GLU:HG2    | 1.73                     | 0.53              |
| 13:n:63:ARG:HE   | 13:n:76:VAL:HG22  | 1.73                     | 0.53              |
| 16:q:58:GLN:O    | 16:q:61:ILE:HG22  | 2.08                     | 0.53              |
| 20:u:64:ILE:HG12 | 20:u:68:ASN:ND2   | 2.23                     | 0.53              |
| 31:G:66:ILE:HA   | 31:G:159:ALA:HB3  | 1.90                     | 0.53              |
| 45:U:40:ASN:CG   | 45:U:43:ALA:HB2   | 2.33                     | 0.53              |
| 49:Y:30:PHE:CZ   | 52:3:1457:G:H5'   | 2.42                     | 0.53              |
| 53:1:1872:A:H2'  | 53:1:1873:G:O4'   | 2.09                     | 0.53              |
| 53:1:2646:C:H2'  | 53:1:2647:U:O4'   | 2.08                     | 0.53              |
| 6:g:2:GLN:O      | 6:g:2:GLN:HG2     | 2.09                     | 0.53              |
| 9:j:37:ARG:HD3   | 9:j:39:LYS:HE2    | 1.91                     | 0.53              |
| 33:I:170:LEU:HG  | 33:I:181:PHE:HA   | 1.91                     | 0.53              |
| 47:W:38:ILE:HG12 | 47:W:58:ILE:HG21  | 1.91                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 51:a:177:LYS:NZ  | 53:1:2125:G:H5'   | 2.24                     | 0.53              |
| 52:3:665:A:O4'   | 52:3:733:G:H1'    | 2.09                     | 0.53              |
| 53:1:621:A:H2'   | 53:1:622:G:H5'    | 1.90                     | 0.53              |
| 53:1:2657:A:H62  | 53:1:2664:G:H21   | 1.54                     | 0.53              |
| 4:e:77:LYS:HD2   | 55:5:57:A:O2'     | 2.09                     | 0.53              |
| 10:k:103:VAL:HB  | 10:k:107:LEU:HD12 | 1.90                     | 0.53              |
| 20:u:84:PHE:HB2  | 53:1:297:G:H5''   | 1.90                     | 0.53              |
| 21:v:35:GLU:HB2  | 21:v:93:ARG:NH1   | 2.23                     | 0.53              |
| 31:G:47:PRO:O    | 31:G:51:GLU:HG2   | 2.09                     | 0.53              |
| 52:3:1277:C:H2'  | 52:3:1278:G:H5''  | 1.91                     | 0.53              |
| 53:1:2118:U:H5   | 53:1:2149:U:H1'   | 1.72                     | 0.53              |
| 6:g:5:LEU:HD22   | 6:g:13:GLY:HA3    | 1.90                     | 0.53              |
| 8:i:7:TYR:HA     | 8:i:58:ILE:O      | 2.08                     | 0.53              |
| 12:m:3:GLN:HE21  | 12:m:92:TRP:NE1   | 2.07                     | 0.53              |
| 17:r:86:GLN:HB3  | 53:1:1225:G:H4'   | 1.91                     | 0.53              |
| 31:G:65:LYS:HG3  | 31:G:157:PRO:HA   | 1.90                     | 0.53              |
| 45:U:21:VAL:HG12 | 45:U:34:GLU:O     | 2.08                     | 0.53              |
| 51:a:27:ILE:HD13 | 51:a:186:LYS:HD2  | 1.91                     | 0.53              |
| 53:1:2799:A:C2'  | 53:1:2800:A:H5'   | 2.39                     | 0.53              |
| 7:h:118:ILE:N    | 7:h:119:PRO:CD    | 2.71                     | 0.53              |
| 11:l:38:GLN:CB   | 53:1:832:U:H5'    | 2.39                     | 0.53              |
| 14:o:90:VAL:HG21 | 14:o:115:LEU:HB3  | 1.91                     | 0.53              |
| 41:Q:35:ARG:HH12 | 41:Q:37:TYR:HB3   | 1.74                     | 0.53              |
| 46:V:64:ARG:HD2  | 52:3:264:C:H4'    | 1.90                     | 0.53              |
| 52:3:86:G:H4'    | 52:3:87:C:C5      | 2.44                     | 0.53              |
| 53:1:1474:U:C2'  | 53:1:1475:G:H5'   | 2.39                     | 0.53              |
| 7:h:54:VAL:HG22  | 7:h:83:ALA:HB1    | 1.91                     | 0.53              |
| 7:h:59:LEU:HD21  | 53:1:1047:G:C8    | 2.43                     | 0.53              |
| 9:j:65:THR:O     | 9:j:68:LYS:HE2    | 2.09                     | 0.53              |
| 12:m:40:ARG:HH11 | 12:m:93:VAL:HG21  | 1.73                     | 0.53              |
| 12:m:108:VAL:HB  | 12:m:112:LEU:HD23 | 1.90                     | 0.53              |
| 25:z:47:ILE:CG2  | 25:z:56:VAL:HG21  | 2.38                     | 0.53              |
| 40:P:93:GLU:HG3  | 40:P:97:ARG:NH1   | 2.24                     | 0.53              |
| 50:Z:11:PHE:C    | 50:Z:13:VAL:H     | 2.17                     | 0.53              |
| 52:3:422:C:H5'   | 52:3:423:G:C2     | 2.43                     | 0.53              |
| 52:3:1251:A:O2'  | 52:3:1370:G:H5'   | 2.09                     | 0.53              |
| 53:1:395:U:H2'   | 53:1:396:G:H8     | 1.75                     | 0.53              |
| 53:1:1790:C:H2'  | 53:1:1791:A:C5    | 2.44                     | 0.53              |
| 53:1:2343:U:H2'  | 53:1:2344:U:C6    | 2.43                     | 0.53              |
| 54:2:28:C:H2'    | 54:2:29:A:C8      | 2.44                     | 0.53              |
| 2:c:33:ARG:HD3   | 2:c:73:VAL:HG22   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:e:39:VAL:HG13   | 4:e:40:GLY:N     | 2.24                     | 0.52              |
| 5:f:94:ARG:HG3    | 5:f:127:GLN:HB2  | 1.89                     | 0.52              |
| 7:h:67:THR:HB     | 7:h:68:PRO:HD3   | 1.91                     | 0.52              |
| 35:K:10:VAL:HG22  | 35:K:11:HIS:N    | 2.24                     | 0.52              |
| 52:3:70:U:H4'     | 52:3:71:A:H8     | 1.73                     | 0.52              |
| 53:1:729:G:H4'    | 53:1:763:G:C5'   | 2.38                     | 0.52              |
| 53:1:1669:A:O3'   | 53:1:2549:G:H5'  | 2.10                     | 0.52              |
| 2:c:155:VAL:O     | 53:1:2619:C:H5'  | 2.09                     | 0.52              |
| 32:H:87:ARG:HE    | 32:H:88:LYS:NZ   | 2.08                     | 0.52              |
| 46:V:16:MET:SD    | 52:3:276:G:H5'   | 2.49                     | 0.52              |
| 52:3:77:A:H2'     | 52:3:78:A:C8     | 2.45                     | 0.52              |
| 53:1:2741:A:H2'   | 53:1:2742:G:O4'  | 2.09                     | 0.52              |
| 1:b:104:LEU:HD23  | 1:b:105:ALA:N    | 2.24                     | 0.52              |
| 1:b:216:ARG:NH2   | 53:1:780:G:H5''  | 2.23                     | 0.52              |
| 5:f:37:ASN:ND2    | 5:f:39:ALA:HB3   | 2.24                     | 0.52              |
| 20:u:27:VAL:HG23  | 20:u:33:VAL:HG12 | 1.91                     | 0.52              |
| 25:z:12:ALA:HA    | 25:z:15:ARG:HD3  | 1.90                     | 0.52              |
| 30:F:1:MET:CE     | 30:F:34:LYS:HZ2  | 2.23                     | 0.52              |
| 34:J:79:THR:OG1   | 34:J:80:LEU:N    | 2.41                     | 0.52              |
| 38:N:110:VAL:HG13 | 38:N:110:VAL:O   | 2.08                     | 0.52              |
| 49:Y:54:GLN:HE21  | 49:Y:75:LYS:HE3  | 1.75                     | 0.52              |
| 53:1:1201:U:H2'   | 53:1:1202:G:H8   | 1.74                     | 0.52              |
| 53:1:2162:G:H2'   | 53:1:2163:A:H8   | 1.73                     | 0.52              |
| 3:d:68:ALA:HA     | 53:1:1255:U:C5   | 2.44                     | 0.52              |
| 12:m:72:PRO:HD3   | 12:m:92:TRP:CZ3  | 2.44                     | 0.52              |
| 14:o:90:VAL:HG23  | 14:o:117:PHE:HB3 | 1.92                     | 0.52              |
| 30:F:17:VAL:HG11  | 53:1:2756:U:OP2  | 2.09                     | 0.52              |
| 32:H:62:SER:OG    | 32:H:97:PRO:HG2  | 2.09                     | 0.52              |
| 39:O:57:VAL:O     | 39:O:58:ASN:HB2  | 2.09                     | 0.52              |
| 40:P:55:ARG:NH2   | 55:6:39:C:H4'    | 2.24                     | 0.52              |
| 43:S:63:CYS:HB3   | 43:S:67:GLY:H    | 1.74                     | 0.52              |
| 50:Z:28:LEU:O     | 50:Z:32:ARG:HG3  | 2.09                     | 0.52              |
| 53:1:2163:A:N3    | 53:1:2163:A:H2'  | 2.25                     | 0.52              |
| 1:b:42:ARG:HH12   | 53:1:691:C:H1'   | 1.75                     | 0.52              |
| 2:c:114:LYS:HD2   | 53:1:2681:C:OP1  | 2.09                     | 0.52              |
| 5:f:44:HIS:O      | 5:f:45:ALA:HB3   | 2.09                     | 0.52              |
| 27:C:21:THR:CG2   | 53:1:2419:U:H5'' | 2.39                     | 0.52              |
| 41:Q:88:ASP:HB2   | 52:3:523:A:H61   | 1.75                     | 0.52              |
| 48:X:39:ILE:HD12  | 48:X:68:HIS:O    | 2.10                     | 0.52              |
| 53:1:2469:A:H2'   | 53:1:2470:G:O4'  | 2.10                     | 0.52              |
| 57:7:14:A:H61     | 57:7:21:A:H2     | 1.56                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:b:58:LYS:O      | 53:1:1568:G:H5'   | 2.10                     | 0.52              |
| 11:l:48:ARG:HH22  | 29:E:4:LYS:HB2    | 1.73                     | 0.52              |
| 28:D:12:ARG:HE    | 28:D:44:VAL:HG21  | 1.74                     | 0.52              |
| 49:Y:2:ASN:ND2    | 52:3:351:G:OP1    | 2.38                     | 0.52              |
| 53:1:1231:U:H2'   | 53:1:1232:G:H8    | 1.74                     | 0.52              |
| 53:1:2104:C:H2'   | 53:1:2105:U:C6    | 2.44                     | 0.52              |
| 53:1:2149:U:H2'   | 53:1:2150:C:O4'   | 2.09                     | 0.52              |
| 54:2:106:G:H2'    | 54:2:107:G:O4'    | 2.08                     | 0.52              |
| 6:g:26:ALA:HA     | 6:g:30:LEU:HD12   | 1.92                     | 0.52              |
| 34:J:112:ALA:O    | 34:J:115:GLU:HG2  | 2.09                     | 0.52              |
| 34:J:148:SER:HB3  | 34:J:151:MET:HG2  | 1.91                     | 0.52              |
| 51:a:10:VAL:O     | 51:a:14:LYS:HG3   | 2.09                     | 0.52              |
| 51:a:63:THR:HG23  | 51:a:163:TYR:HE1  | 1.75                     | 0.52              |
| 53:1:1983:G:H4'   | 53:1:2606:C:H4'   | 1.92                     | 0.52              |
| 53:1:2676:C:H2'   | 53:1:2677:G:C8    | 2.45                     | 0.52              |
| 1:b:52:HIS:CE1    | 1:b:218:THR:HG22  | 2.45                     | 0.52              |
| 10:k:1:MET:HE1    | 53:1:2726:A:O3'   | 2.10                     | 0.52              |
| 13:n:2:ARG:HA     | 13:n:5:LYS:HD2    | 1.90                     | 0.52              |
| 32:H:172:VAL:HG23 | 52:3:1107:C:C5'   | 2.40                     | 0.52              |
| 34:J:156:ARG:HH12 | 37:M:100:ILE:HG23 | 1.74                     | 0.52              |
| 52:3:1412:C:H2'   | 52:3:1413:A:C8    | 2.44                     | 0.52              |
| 53:1:2423:U:HO2'  | 53:1:2425:A:H2'   | 1.75                     | 0.52              |
| 5:f:16:VAL:HG21   | 5:f:44:HIS:CE1    | 2.45                     | 0.52              |
| 13:n:92:GLY:O     | 53:1:2880:C:H1'   | 2.10                     | 0.52              |
| 33:I:98:ASP:N     | 33:I:132:ALA:O    | 2.43                     | 0.52              |
| 34:J:44:ARG:HA    | 34:J:72:ASN:HA    | 1.91                     | 0.52              |
| 36:L:76:SER:OG    | 55:6:33:U:H5'     | 2.10                     | 0.52              |
| 37:M:77:VAL:HG23  | 37:M:126:CYS:HA   | 1.92                     | 0.52              |
| 52:3:927:G:H21    | 52:3:1532:U:H5''  | 1.75                     | 0.52              |
| 52:3:1202:U:C2'   | 52:3:1203:C:H5'   | 2.40                     | 0.52              |
| 53:1:1979:U:O2'   | 53:1:1980:G:H5'   | 2.09                     | 0.52              |
| 1:b:220:ARG:HH12  | 1:b:237:ARG:NH2   | 2.08                     | 0.52              |
| 10:k:1:MET:HG3    | 10:k:32:TYR:HB3   | 1.91                     | 0.52              |
| 11:l:96:LYS:HG3   | 11:l:101:ILE:HD11 | 1.91                     | 0.52              |
| 12:m:10:ARG:HG3   | 12:m:11:LYS:HG2   | 1.91                     | 0.52              |
| 32:H:111:ASP:OD2  | 32:H:114:LEU:HG   | 2.10                     | 0.52              |
| 35:K:38:ARG:O     | 35:K:39:LEU:HD22  | 2.10                     | 0.52              |
| 41:Q:29:LYS:HD3   | 52:3:363:A:P      | 2.49                     | 0.52              |
| 41:Q:50:LYS:HD2   | 41:Q:50:LYS:N     | 2.25                     | 0.52              |
| 53:1:1023:U:O2'   | 53:1:1122:G:H5'   | 2.09                     | 0.52              |
| 53:1:1474:U:H2'   | 53:1:1475:G:H5'   | 1.92                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:2372:U:H2'  | 53:1:2373:G:C8    | 2.45                     | 0.52              |
| 53:1:2372:U:H2'  | 53:1:2373:G:H8    | 1.75                     | 0.52              |
| 4:e:102:LEU:HA   | 4:e:106:ALA:HB3   | 1.91                     | 0.51              |
| 7:h:40:GLU:O     | 7:h:43:LYS:HB3    | 2.11                     | 0.51              |
| 10:k:7:MET:SD    | 10:k:20:MET:HE2   | 2.50                     | 0.51              |
| 14:o:88:LYS:HG3  | 14:o:116:GLN:HE21 | 1.75                     | 0.51              |
| 16:q:52:ARG:HG2  | 53:1:995:C:H5''   | 1.92                     | 0.51              |
| 20:u:90:LYS:HE2  | 53:1:101:A:N6     | 2.24                     | 0.51              |
| 34:J:56:PRO:O    | 34:J:59:ILE:HG22  | 2.10                     | 0.51              |
| 53:1:2048:G:C2'  | 53:1:2049:G:H5''  | 2.40                     | 0.51              |
| 53:1:2141:G:H22  | 53:1:2151:U:H1'   | 1.74                     | 0.51              |
| 53:1:2183:A:H2'  | 53:1:2184:A:C8    | 2.45                     | 0.51              |
| 53:1:2350:C:H2'  | 53:1:2351:G:O4'   | 2.10                     | 0.51              |
| 53:1:2467:C:H2'  | 53:1:2468:A:O4'   | 2.10                     | 0.51              |
| 1:b:226:PRO:HG3  | 1:b:232:GLY:C     | 2.35                     | 0.51              |
| 3:d:149:ILE:HD11 | 3:d:172:ALA:HA    | 1.92                     | 0.51              |
| 21:v:78:GLN:NE2  | 54:2:76:G:H21     | 2.09                     | 0.51              |
| 32:H:64:ARG:HH11 | 32:H:99:GLN:H     | 1.59                     | 0.51              |
| 48:X:22:VAL:HG13 | 48:X:23:GLU:OE1   | 2.10                     | 0.51              |
| 53:1:713:G:H21   | 53:1:718:A:H62    | 1.56                     | 0.51              |
| 56:4:20:U:H2'    | 56:4:21:C:C6      | 2.45                     | 0.51              |
| 2:c:46:ARG:HB2   | 2:c:84:LEU:HD12   | 1.92                     | 0.51              |
| 2:c:47:ALA:HA    | 2:c:84:LEU:H      | 1.76                     | 0.51              |
| 2:c:161:MET:HE1  | 53:1:2050:C:O2    | 2.10                     | 0.51              |
| 34:J:37:VAL:HG21 | 34:J:113:VAL:HG12 | 1.91                     | 0.51              |
| 41:Q:119:LYS:CG  | 52:3:36:C:H5''    | 2.39                     | 0.51              |
| 52:3:959:A:H2'   | 52:3:960:U:H4'    | 1.92                     | 0.51              |
| 53:1:1380:G:H1'  | 53:1:1569:A:H61   | 1.76                     | 0.51              |
| 7:h:33:VAL:HB    | 7:h:35:VAL:HG22   | 1.92                     | 0.51              |
| 16:q:48:ASP:HA   | 16:q:51:GLN:HB2   | 1.91                     | 0.51              |
| 29:E:51:LYS:HD2  | 29:E:54:LEU:HD12  | 1.92                     | 0.51              |
| 50:Z:28:LEU:HA   | 50:Z:31:VAL:HG22  | 1.93                     | 0.51              |
| 51:a:7:ARG:NH2   | 51:a:35:THR:HB    | 2.24                     | 0.51              |
| 52:3:1319:A:H4'  | 52:3:1320:C:H5    | 1.76                     | 0.51              |
| 53:1:441:U:H2'   | 53:1:442:G:C8     | 2.45                     | 0.51              |
| 54:2:88:C:H4'    | 54:2:89:U:OP1     | 2.10                     | 0.51              |
| 4:e:42:ALA:HB3   | 4:e:84:ILE:HG23   | 1.93                     | 0.51              |
| 8:i:6:ALA:O      | 8:i:30:GLN:HG2    | 2.11                     | 0.51              |
| 9:j:96:ARG:NH1   | 53:1:2639:A:H5''  | 2.21                     | 0.51              |
| 40:P:49:SER:HB3  | 40:P:68:ARG:HD2   | 1.91                     | 0.51              |
| 52:3:1316:G:H2'  | 52:3:1317:C:H5''  | 1.92                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 53:1:2343:U:O2'   | 53:1:2344:U:H5'  | 2.10                     | 0.51              |
| 53:1:2724:U:H2'   | 53:1:2725:A:C8   | 2.45                     | 0.51              |
| 2:c:33:ARG:HD3    | 2:c:73:VAL:CG2   | 2.40                     | 0.51              |
| 9:j:8:PRO:HG3     | 9:j:48:VAL:HG13  | 1.93                     | 0.51              |
| 9:j:42:ALA:O      | 16:q:63:ARG:HD2  | 2.10                     | 0.51              |
| 16:q:73:ILE:N     | 16:q:73:ILE:HD12 | 2.25                     | 0.51              |
| 22:w:15:LYS:HG3   | 22:w:37:ARG:HH22 | 1.75                     | 0.51              |
| 23:x:56:ARG:NH2   | 53:1:399:U:OP2   | 2.43                     | 0.51              |
| 29:E:61:LEU:HB2   | 29:E:64:ALA:HB3  | 1.91                     | 0.51              |
| 31:G:52:ALA:O     | 31:G:56:LEU:HD23 | 2.11                     | 0.51              |
| 32:H:18:ASN:ND2   | 43:S:89:ARG:O    | 2.44                     | 0.51              |
| 32:H:31:ASN:HD22  | 32:H:58:ARG:NH1  | 2.09                     | 0.51              |
| 36:L:102:TRP:CD1  | 36:L:136:LYS:HG2 | 2.46                     | 0.51              |
| 40:P:85:VAL:HG23  | 40:P:111:ASP:HA  | 1.93                     | 0.51              |
| 41:Q:86:VAL:HG12  | 41:Q:95:HIS:NE2  | 2.26                     | 0.51              |
| 42:R:89:ARG:HH21  | 42:R:95:PRO:HG2  | 1.74                     | 0.51              |
| 51:a:181:ASP:HB3  | 51:a:184:LYS:HD3 | 1.93                     | 0.51              |
| 52:3:483:C:H2'    | 52:3:484:G:C8    | 2.46                     | 0.51              |
| 54:2:49:C:H2'     | 54:2:50:A:C8     | 2.45                     | 0.51              |
| 3:d:119:ILE:HB    | 3:d:187:VAL:HA   | 1.92                     | 0.51              |
| 14:o:25:ARG:HA    | 14:o:91:SER:OG   | 2.11                     | 0.51              |
| 24:y:41:HIS:CE1   | 53:1:96:C:H4'    | 2.46                     | 0.51              |
| 25:z:8:GLN:HB2    | 25:z:28:LEU:HD22 | 1.92                     | 0.51              |
| 26:B:9:ARG:H      | 26:B:9:ARG:HD2   | 1.75                     | 0.51              |
| 39:O:100:ILE:HD12 | 39:O:100:ILE:N   | 2.26                     | 0.51              |
| 47:W:25:ILE:HA    | 47:W:28:LEU:HB3  | 1.92                     | 0.51              |
| 52:3:1105:A:H2'   | 52:3:1106:G:H8   | 1.75                     | 0.51              |
| 54:2:65:U:H3'     | 54:2:108:A:H61   | 1.74                     | 0.51              |
| 4:e:48:LEU:HD21   | 4:e:147:ARG:HH12 | 1.76                     | 0.51              |
| 5:f:16:VAL:HG21   | 5:f:44:HIS:HE1   | 1.75                     | 0.51              |
| 13:n:96:ARG:HH11  | 53:1:2881:U:H5'' | 1.75                     | 0.51              |
| 18:s:49:LYS:HD3   | 53:1:492:A:N1    | 2.25                     | 0.51              |
| 28:D:14:ARG:HG2   | 53:1:125:A:H5'   | 1.91                     | 0.51              |
| 33:I:156:ALA:O    | 33:I:159:GLU:HG3 | 2.11                     | 0.51              |
| 39:O:22:THR:O     | 39:O:25:ILE:HG22 | 2.11                     | 0.51              |
| 39:O:68:ARG:HH22  | 52:3:1115:U:H5'  | 1.75                     | 0.51              |
| 41:Q:49:ARG:HH12  | 52:3:521:G:H5''  | 1.76                     | 0.51              |
| 52:3:1130:A:H61   | 52:3:1144:G:H1'  | 1.75                     | 0.51              |
| 1:b:220:ARG:HD3   | 53:1:1827:U:H5   | 1.76                     | 0.51              |
| 18:s:25:ARG:O     | 18:s:25:ARG:HD3  | 2.10                     | 0.51              |
| 23:x:29:LEU:HD12  | 23:x:30:PRO:CD   | 2.40                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 28:D:1:MET:HE1   | 53:1:789:A:C2    | 2.46                     | 0.51              |
| 37:M:63:LYS:HE2  | 37:M:70:VAL:HG21 | 1.93                     | 0.51              |
| 38:N:121:ARG:HB3 | 52:3:1344:C:H4'  | 1.93                     | 0.51              |
| 39:O:5:ARG:HB3   | 39:O:6:ILE:HD12  | 1.92                     | 0.51              |
| 52:3:372:C:N4    | 52:3:387:U:H2'   | 2.26                     | 0.51              |
| 52:3:1261:A:H1'  | 52:3:1283:U:H5'' | 1.92                     | 0.51              |
| 53:1:1035:U:H2'  | 53:1:1036:G:H8   | 1.76                     | 0.51              |
| 54:2:35:C:H2'    | 54:2:36:C:H5'    | 1.93                     | 0.51              |
| 1:b:45:ASN:O     | 53:1:773:U:H4'   | 2.10                     | 0.51              |
| 8:i:57:VAL:HB    | 8:i:69:VAL:HB    | 1.93                     | 0.51              |
| 34:J:92:ARG:O    | 34:J:93:VAL:C    | 2.54                     | 0.51              |
| 35:K:11:HIS:ND1  | 35:K:12:PRO:HD2  | 2.26                     | 0.51              |
| 42:R:65:GLU:CD   | 42:R:65:GLU:H    | 2.19                     | 0.51              |
| 52:3:945:G:H2'   | 52:3:945:G:N3    | 2.25                     | 0.51              |
| 52:3:1237:C:OP1  | 52:3:1238:A:H1'  | 2.10                     | 0.51              |
| 27:C:7:LYS:HA    | 27:C:23:THR:HA   | 1.91                     | 0.50              |
| 40:P:91:GLY:C    | 40:P:93:GLU:H    | 2.19                     | 0.50              |
| 52:3:335:C:H2'   | 52:3:336:A:C8    | 2.45                     | 0.50              |
| 53:1:473:G:O2'   | 53:1:474:G:H5'   | 2.11                     | 0.50              |
| 53:1:2112:G:H2'  | 53:1:2113:U:H5'  | 1.93                     | 0.50              |
| 53:1:2757:A:H2'  | 53:1:2757:A:N3   | 2.26                     | 0.50              |
| 16:q:8:ILE:HG23  | 16:q:9:ALA:N     | 2.26                     | 0.50              |
| 52:3:494:G:O2'   | 52:3:496:A:H1'   | 2.10                     | 0.50              |
| 52:3:1497:G:O2'  | 52:3:1498:U:H5'  | 2.11                     | 0.50              |
| 53:1:1297:C:H2'  | 53:1:1298:C:C6   | 2.47                     | 0.50              |
| 53:1:2285:C:O2'  | 53:1:2287:A:H1'  | 2.11                     | 0.50              |
| 3:d:59:PRO:HB2   | 3:d:60:TRP:CE3   | 2.46                     | 0.50              |
| 4:e:110:ILE:HB   | 4:e:113:PHE:HB2  | 1.92                     | 0.50              |
| 7:h:50:VAL:HG22  | 7:h:50:VAL:O     | 2.12                     | 0.50              |
| 7:h:94:ARG:HH21  | 7:h:131:THR:HA   | 1.76                     | 0.50              |
| 10:k:87:LEU:HB3  | 10:k:92:GLU:O    | 2.10                     | 0.50              |
| 35:K:49:TYR:OH   | 35:K:86:ARG:NH1  | 2.44                     | 0.50              |
| 38:N:89:TYR:HB3  | 38:N:93:LEU:HD12 | 1.94                     | 0.50              |
| 39:O:83:THR:HG22 | 39:O:87:LEU:HG   | 1.93                     | 0.50              |
| 40:P:44:ALA:HB1  | 40:P:68:ARG:HG3  | 1.92                     | 0.50              |
| 52:3:1402:C:H2'  | 52:3:1403:C:O4'  | 2.11                     | 0.50              |
| 53:1:582:A:H2'   | 53:1:583:G:C8    | 2.45                     | 0.50              |
| 53:1:1810:A:H2'  | 53:1:1811:G:O4'  | 2.11                     | 0.50              |
| 53:1:2139:U:H2'  | 53:1:2140:G:C8   | 2.46                     | 0.50              |
| 53:1:2257:U:O2'  | 53:1:2258:C:H5'  | 2.11                     | 0.50              |
| 53:1:2463:C:H2'  | 53:1:2464:G:H8   | 1.77                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:b:77:VAL:HG11   | 1:b:109:LEU:HD11  | 1.94                     | 0.50              |
| 1:b:212:TRP:HE1   | 1:b:213:ARG:HH12  | 1.60                     | 0.50              |
| 8:i:91:LYS:HB3    | 8:i:94:LYS:HB2    | 1.92                     | 0.50              |
| 9:j:106:LYS:NZ    | 9:j:116:ARG:HG2   | 2.27                     | 0.50              |
| 16:q:12:ARG:HH22  | 53:1:812:C:H4'    | 1.77                     | 0.50              |
| 17:r:38:VAL:HG11  | 17:r:57:GLY:HA3   | 1.92                     | 0.50              |
| 28:D:26:ASN:OD1   | 53:1:682:G:H5'    | 2.11                     | 0.50              |
| 38:N:18:VAL:HG12  | 38:N:64:ILE:HG22  | 1.92                     | 0.50              |
| 41:Q:41:PRO:HD2   | 41:Q:47:ALA:H     | 1.76                     | 0.50              |
| 43:S:81:ILE:HG21  | 52:3:1202:U:N3    | 2.26                     | 0.50              |
| 53:1:532:A:H2'    | 53:1:532:A:N3     | 2.27                     | 0.50              |
| 53:1:2156:G:C2'   | 53:1:2157:G:H5'   | 2.41                     | 0.50              |
| 3:d:2:GLU:HB3     | 3:d:11:ALA:HB1    | 1.94                     | 0.50              |
| 5:f:15:ASP:HB2    | 5:f:26:LYS:HB3    | 1.93                     | 0.50              |
| 5:f:91:VAL:HG13   | 5:f:94:ARG:HH12   | 1.76                     | 0.50              |
| 6:g:4:ILE:HG13    | 6:g:39:ALA:HB2    | 1.94                     | 0.50              |
| 10:k:35:VAL:HG11  | 10:k:106:GLU:OE1  | 2.12                     | 0.50              |
| 14:o:34:HIS:ND1   | 14:o:53:THR:HG23  | 2.25                     | 0.50              |
| 18:s:78:GLU:HA    | 18:s:101:SER:HA   | 1.92                     | 0.50              |
| 31:G:107:ARG:O    | 31:G:111:LYS:HG3  | 2.12                     | 0.50              |
| 33:I:124:VAL:HG22 | 33:I:142:VAL:HG12 | 1.92                     | 0.50              |
| 40:P:32:THR:HG22  | 40:P:43:TRP:HB3   | 1.94                     | 0.50              |
| 53:1:1856:U:H2'   | 53:1:1857:G:O4'   | 2.12                     | 0.50              |
| 3:d:117:ARG:HH12  | 11:l:2:ARG:NH2    | 2.06                     | 0.50              |
| 8:i:9:LYS:HG2     | 8:i:57:VAL:HG22   | 1.94                     | 0.50              |
| 10:k:22:ILE:HG12  | 10:k:40:LYS:O     | 2.11                     | 0.50              |
| 11:l:93:ASN:O     | 11:l:94:THR:OG1   | 2.25                     | 0.50              |
| 16:q:27:ARG:HD2   | 53:1:533:G:OP1    | 2.12                     | 0.50              |
| 18:s:11:ARG:HH22  | 18:s:98:LYS:HB3   | 1.75                     | 0.50              |
| 42:R:77:LYS:HZ2   | 42:R:80:MET:HE3   | 1.76                     | 0.50              |
| 48:X:62:THR:OG1   | 48:X:65:MET:HE3   | 2.11                     | 0.50              |
| 51:a:196:LEU:HD21 | 51:a:209:ILE:HD12 | 1.93                     | 0.50              |
| 52:3:948:C:H2'    | 52:3:949:A:C8     | 2.47                     | 0.50              |
| 53:1:1357:C:H2'   | 53:1:1358:G:O4'   | 2.12                     | 0.50              |
| 53:1:2577:A:H2'   | 53:1:2614:A:N6    | 2.26                     | 0.50              |
| 6:g:21:VAL:HG22   | 6:g:22:LYS:N      | 2.27                     | 0.50              |
| 7:h:58:THR:HA     | 7:h:63:ALA:HB2    | 1.93                     | 0.50              |
| 30:F:36:ARG:HH22  | 53:1:2742:G:H5'   | 1.76                     | 0.50              |
| 32:H:141:MET:HE3  | 32:H:169:GLU:HG3  | 1.94                     | 0.50              |
| 33:I:31:CYS:HA    | 52:3:429:U:OP2    | 2.11                     | 0.50              |
| 34:J:133:ILE:HG13 | 52:3:1078:U:O2'   | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:W:54:LEU:O     | 47:W:58:ILE:HG12  | 2.12                     | 0.50              |
| 51:a:170:ILE:HD12 | 51:a:170:ILE:H    | 1.76                     | 0.50              |
| 52:3:235:C:H2'    | 52:3:236:A:H8     | 1.75                     | 0.50              |
| 52:3:1280:A:O2'   | 52:3:1281:C:H5'   | 2.12                     | 0.50              |
| 52:3:1323:G:H2'   | 52:3:1324:A:C8    | 2.47                     | 0.50              |
| 53:1:937:C:H2'    | 53:1:938:G:C8     | 2.47                     | 0.50              |
| 53:1:1268:A:H2'   | 53:1:1269:A:O4'   | 2.12                     | 0.50              |
| 53:1:1378:A:H1'   | 53:1:1379:U:C5    | 2.46                     | 0.50              |
| 5:f:22:VAL:HA     | 5:f:35:THR:HA     | 1.94                     | 0.50              |
| 6:g:51:ARG:HA     | 6:g:55:GLU:HB2    | 1.93                     | 0.50              |
| 10:k:34:GLY:H     | 10:k:37:ASP:HB2   | 1.76                     | 0.50              |
| 17:r:69:GLY:N     | 17:r:91:GLN:O     | 2.45                     | 0.50              |
| 20:u:71:ILE:HD12  | 20:u:71:ILE:N     | 2.27                     | 0.50              |
| 28:D:34:ARG:HH12  | 53:1:466:A:P      | 2.34                     | 0.50              |
| 52:3:1527:U:O2'   | 52:3:1528:U:H5'   | 2.11                     | 0.50              |
| 53:1:506:G:H4'    | 53:1:509:C:H1'    | 1.94                     | 0.50              |
| 54:2:2:G:H2'      | 54:2:3:C:C6       | 2.46                     | 0.50              |
| 1:b:38:LYS:HE3    | 1:b:53:ILE:HD11   | 1.93                     | 0.50              |
| 1:b:213:ARG:NH1   | 53:1:1566:A:H5'   | 2.27                     | 0.50              |
| 8:i:55:PRO:HD3    | 8:i:74:PRO:HD3    | 1.94                     | 0.50              |
| 16:q:5:ARG:HH22   | 53:1:1251:C:H5    | 1.60                     | 0.50              |
| 18:s:42:LYS:HD3   | 53:1:2010:G:O3'   | 2.12                     | 0.50              |
| 38:N:8:THR:HG23   | 52:3:1148:U:H5''  | 1.93                     | 0.50              |
| 52:3:1308:U:H2'   | 52:3:1309:G:H8    | 1.76                     | 0.50              |
| 52:3:1512:U:H2'   | 52:3:1513:A:C8    | 2.46                     | 0.50              |
| 11:l:56:PRO:O     | 11:l:60:ARG:HG3   | 2.12                     | 0.49              |
| 22:w:47:VAL:HB    | 22:w:55:LEU:HD12  | 1.93                     | 0.49              |
| 32:H:26:LYS:HZ1   | 52:3:1278:G:H8    | 1.55                     | 0.49              |
| 33:I:99:ASN:HA    | 33:I:110:ARG:HH12 | 1.77                     | 0.49              |
| 33:I:170:LEU:HD23 | 33:I:171:GLU:N    | 2.27                     | 0.49              |
| 52:3:880:C:H2'    | 52:3:881:G:H8     | 1.76                     | 0.49              |
| 53:1:558:U:H2'    | 53:1:559:G:H8     | 1.77                     | 0.49              |
| 53:1:1535:A:H3'   | 53:1:1536:C:H5'   | 1.94                     | 0.49              |
| 53:1:2628:C:H3'   | 53:1:2629:U:H5'   | 1.93                     | 0.49              |
| 54:2:49:C:H2'     | 54:2:50:A:H8      | 1.77                     | 0.49              |
| 4:e:23:SER:HB3    | 4:e:26:GLN:HG3    | 1.95                     | 0.49              |
| 9:j:35:ARG:HA     | 9:j:40:HIS:HD2    | 1.76                     | 0.49              |
| 15:p:13:LYS:HG2   | 15:p:76:HIS:ND1   | 2.27                     | 0.49              |
| 26:B:5:ASN:ND2    | 53:1:2020:A:H62   | 2.10                     | 0.49              |
| 37:M:29:SER:HB3   | 37:M:32:LYS:HG3   | 1.94                     | 0.49              |
| 52:3:758:C:H4'    | 52:3:880:C:H4'    | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:1:581:C:H2'   | 53:1:582:A:C8    | 2.47                     | 0.49              |
| 53:1:1162:G:H2'  | 53:1:1163:G:H8   | 1.77                     | 0.49              |
| 53:1:1991:U:H2'  | 53:1:1992:G:H5'' | 1.94                     | 0.49              |
| 11:l:77:ILE:HD13 | 11:l:108:ALA:HB1 | 1.94                     | 0.49              |
| 18:s:74:ILE:HG23 | 18:s:74:ILE:O    | 2.13                     | 0.49              |
| 35:K:9:MET:HA    | 35:K:58:HIS:O    | 2.12                     | 0.49              |
| 41:Q:43:LYS:HZ1  | 56:4:20:U:C4'    | 2.24                     | 0.49              |
| 45:U:13:LYS:HE2  | 52:3:392:C:H5'   | 1.94                     | 0.49              |
| 50:Z:5:VAL:HG11  | 50:Z:16:ARG:HA   | 1.93                     | 0.49              |
| 53:1:1418:G:H21  | 53:1:1580:A:H62  | 1.60                     | 0.49              |
| 53:1:1554:U:H3'  | 53:1:1555:G:H5'  | 1.92                     | 0.49              |
| 12:m:40:ARG:NH1  | 12:m:93:VAL:HG21 | 2.27                     | 0.49              |
| 16:q:5:ARG:NH2   | 53:1:1251:C:H5   | 2.10                     | 0.49              |
| 19:t:39:THR:HG22 | 19:t:42:GLU:HB2  | 1.95                     | 0.49              |
| 21:v:70:ILE:HD12 | 21:v:70:ILE:N    | 2.27                     | 0.49              |
| 26:B:9:ARG:HD2   | 26:B:9:ARG:N     | 2.28                     | 0.49              |
| 39:O:14:ASP:OD2  | 39:O:16:ARG:HG2  | 2.11                     | 0.49              |
| 40:P:52:ARG:HA   | 40:P:56:LYS:HG3  | 1.93                     | 0.49              |
| 52:3:1497:G:C2'  | 52:3:1498:U:H5'  | 2.42                     | 0.49              |
| 38:N:105:ARG:HD2 | 52:3:1117:A:O2'  | 2.12                     | 0.49              |
| 46:V:45:VAL:HG13 | 46:V:73:THR:C    | 2.38                     | 0.49              |
| 52:3:1259:C:H3'  | 52:3:1260:G:C5'  | 2.39                     | 0.49              |
| 53:1:225:C:H2'   | 53:1:226:A:O4'   | 2.13                     | 0.49              |
| 53:1:1060:U:H4'  | 53:1:1061:U:H5'  | 1.95                     | 0.49              |
| 7:h:55:VAL:HG22  | 53:1:1084:A:O5'  | 2.13                     | 0.49              |
| 7:h:56:ARG:NH1   | 7:h:83:ALA:HB2   | 2.28                     | 0.49              |
| 32:H:64:ARG:NH1  | 32:H:99:GLN:H    | 2.10                     | 0.49              |
| 34:J:24:VAL:HG22 | 34:J:25:LYS:N    | 2.24                     | 0.49              |
| 35:K:12:PRO:O    | 35:K:15:SER:HB2  | 2.12                     | 0.49              |
| 49:Y:66:ILE:HG22 | 49:Y:68:LYS:H    | 1.77                     | 0.49              |
| 52:3:113:G:H2'   | 52:3:114:U:C6    | 2.47                     | 0.49              |
| 52:3:1060:U:H2'  | 52:3:1061:G:H8   | 1.77                     | 0.49              |
| 53:1:616:A:H2'   | 53:1:617:G:O4'   | 2.11                     | 0.49              |
| 53:1:996:A:H2'   | 53:1:997:G:C8    | 2.47                     | 0.49              |
| 53:1:1170:C:H2'  | 53:1:1171:G:C8   | 2.48                     | 0.49              |
| 53:1:1683:U:H2'  | 53:1:1684:G:C8   | 2.48                     | 0.49              |
| 7:h:13:ALA:HB3   | 7:h:53:ARG:HH12  | 1.78                     | 0.49              |
| 34:J:108:GLY:H   | 52:3:9:G:C5'     | 2.26                     | 0.49              |
| 44:T:56:LEU:HD11 | 53:1:715:A:N6    | 2.28                     | 0.49              |
| 52:3:45:G:H5''   | 52:3:307:C:O2'   | 2.12                     | 0.49              |
| 52:3:730:G:H2'   | 52:3:731:G:H5'   | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:1882:U:H2'   | 53:1:1883:U:C6    | 2.48                     | 0.49              |
| 1:b:104:LEU:HD21  | 1:b:194:VAL:HG13  | 1.94                     | 0.49              |
| 1:b:181:ARG:HB3   | 1:b:181:ARG:CZ    | 2.43                     | 0.49              |
| 2:c:24:VAL:HG21   | 2:c:188:LEU:HB3   | 1.95                     | 0.49              |
| 5:f:163:TYR:HB2   | 5:f:166:GLU:HB2   | 1.94                     | 0.49              |
| 31:G:11:ALA:HB1   | 31:G:208:ALA:HA   | 1.94                     | 0.49              |
| 43:S:52:ARG:HG2   | 52:3:1219:A:OP1   | 2.13                     | 0.49              |
| 45:U:44:SER:H     | 45:U:46:LYS:HZ1   | 1.60                     | 0.49              |
| 52:3:1201:A:C1'   | 52:3:1202:U:OP2   | 2.57                     | 0.49              |
| 53:1:2086:U:H2'   | 53:1:2087:G:C8    | 2.47                     | 0.49              |
| 53:1:2515:C:H2'   | 53:1:2516:A:H8    | 1.78                     | 0.49              |
| 6:g:8:LYS:HD2     | 6:g:8:LYS:C       | 2.37                     | 0.49              |
| 9:j:53:TYR:HA     | 9:j:121:LYS:HB3   | 1.94                     | 0.49              |
| 20:u:14:THR:HA    | 20:u:18:LYS:HG3   | 1.95                     | 0.49              |
| 26:B:3:GLN:HA     | 53:1:2615:U:C2    | 2.48                     | 0.49              |
| 26:B:39:ARG:HD3   | 53:1:2886:A:N1    | 2.27                     | 0.49              |
| 32:H:120:THR:HG23 | 32:H:188:ALA:HA   | 1.95                     | 0.49              |
| 32:H:168:ARG:HH12 | 52:3:1106:G:H21   | 1.61                     | 0.49              |
| 39:O:49:PHE:HB2   | 39:O:65:TYR:HB2   | 1.94                     | 0.49              |
| 40:P:87:GLY:H     | 40:P:113:THR:HG22 | 1.77                     | 0.49              |
| 41:Q:88:ASP:O     | 41:Q:89:LEU:HD22  | 2.12                     | 0.49              |
| 51:a:39:VAL:HG22  | 51:a:177:LYS:HD2  | 1.94                     | 0.49              |
| 53:1:807:U:H2'    | 53:1:808:G:H8     | 1.77                     | 0.49              |
| 53:1:818:G:O2'    | 53:1:819:A:H5''   | 2.13                     | 0.49              |
| 53:1:910:A:H2'    | 53:1:911:A:C8     | 2.48                     | 0.49              |
| 53:1:1525:A:H2'   | 53:1:1526:C:O4'   | 2.12                     | 0.49              |
| 3:d:57:LYS:O      | 3:d:57:LYS:HD2    | 2.13                     | 0.49              |
| 3:d:153:LEU:O     | 3:d:153:LEU:HD12  | 2.13                     | 0.49              |
| 7:h:47:GLU:OE1    | 7:h:52:MET:HG3    | 2.13                     | 0.49              |
| 11:l:46:VAL:HB    | 11:l:50:PHE:HB3   | 1.95                     | 0.49              |
| 19:t:61:LEU:CD1   | 53:1:1340:U:H2'   | 2.37                     | 0.49              |
| 27:C:16:THR:HG21  | 27:C:39:ASP:OD2   | 2.13                     | 0.49              |
| 33:I:78:ALA:CB    | 33:I:85:THR:HG23  | 2.43                     | 0.49              |
| 36:L:38:ALA:HA    | 36:L:41:ILE:HD12  | 1.93                     | 0.49              |
| 37:M:83:ARG:NH2   | 52:3:643:C:O2'    | 2.46                     | 0.49              |
| 40:P:39:ASN:HD22  | 52:3:683:G:H21    | 1.60                     | 0.49              |
| 40:P:85:VAL:HG21  | 50:Z:16:ARG:HH22  | 1.78                     | 0.49              |
| 41:Q:33:CYS:HA    | 41:Q:54:VAL:HA    | 1.95                     | 0.49              |
| 49:Y:67:HIS:HE1   | 52:3:132:C:H4'    | 1.77                     | 0.49              |
| 51:a:27:ILE:HG21  | 51:a:186:LYS:HB2  | 1.95                     | 0.49              |
| 52:3:396:C:C3'    | 52:3:397:A:H5''   | 2.43                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:3:1391:U:H2'   | 52:3:1392:G:C8    | 2.48                     | 0.49              |
| 53:1:20:C:H2'     | 53:1:21:A:C8      | 2.47                     | 0.49              |
| 53:1:326:G:H2'    | 53:1:327:G:C8     | 2.48                     | 0.49              |
| 53:1:1547:C:H2'   | 53:1:1548:A:C8    | 2.48                     | 0.49              |
| 53:1:2443:C:H2'   | 53:1:2444:G:C8    | 2.48                     | 0.49              |
| 1:b:175:LEU:HD12  | 1:b:179:GLU:HB3   | 1.94                     | 0.48              |
| 2:c:133:THR:OG1   | 2:c:134:HIS:N     | 2.37                     | 0.48              |
| 5:f:26:LYS:HB2    | 5:f:31:GLU:OE2    | 2.12                     | 0.48              |
| 10:k:37:ASP:OD1   | 10:k:39:ILE:HG23  | 2.12                     | 0.48              |
| 11:l:68:SER:HB3   | 11:l:71:ALA:HB2   | 1.95                     | 0.48              |
| 11:l:90:VAL:HB    | 11:l:122:VAL:HA   | 1.94                     | 0.48              |
| 16:q:12:ARG:NH1   | 53:1:812:C:H4'    | 2.26                     | 0.48              |
| 22:w:16:ARG:HD2   | 53:1:2356:U:H4'   | 1.93                     | 0.48              |
| 32:H:159:ALA:HB3  | 32:H:163:ARG:NH1  | 2.27                     | 0.48              |
| 34:J:105:ILE:HG13 | 34:J:105:ILE:O    | 2.12                     | 0.48              |
| 39:O:12:ALA:HB3   | 39:O:18:ILE:CG2   | 2.43                     | 0.48              |
| 47:W:53:GLN:HG2   | 47:W:56:ARG:HE    | 1.78                     | 0.48              |
| 53:1:639:U:H2'    | 53:1:640:C:C6     | 2.48                     | 0.48              |
| 55:6:72:A:H2'     | 55:6:73:A:O4'     | 2.13                     | 0.48              |
| 2:c:127:PHE:CE2   | 53:1:2512:C:H4'   | 2.47                     | 0.48              |
| 9:j:47:HIS:ND1    | 9:j:48:VAL:HG23   | 2.28                     | 0.48              |
| 10:k:104:THR:H    | 10:k:107:LEU:HD12 | 1.78                     | 0.48              |
| 16:q:32:ARG:NE    | 53:1:581:C:OP2    | 2.45                     | 0.48              |
| 20:u:97:SER:O     | 20:u:98:ASN:HB2   | 2.13                     | 0.48              |
| 40:P:20:ALA:HA    | 40:P:33:ILE:HA    | 1.95                     | 0.48              |
| 44:T:62:ARG:O     | 44:T:66:LEU:HG    | 2.14                     | 0.48              |
| 45:U:14:ARG:NH1   | 52:3:618:C:H1'    | 2.29                     | 0.48              |
| 46:V:71:SER:OG    | 52:3:235:C:H4'    | 2.13                     | 0.48              |
| 52:3:918:A:H2'    | 52:3:919:A:O4'    | 2.13                     | 0.48              |
| 53:1:1001:A:H2'   | 53:1:1002:G:O4'   | 2.13                     | 0.48              |
| 53:1:1807:G:H2'   | 53:1:1808:A:H5'   | 1.95                     | 0.48              |
| 53:1:2087:G:H2'   | 53:1:2088:A:H8    | 1.76                     | 0.48              |
| 53:1:2358:A:H2'   | 53:1:2359:C:O4'   | 2.13                     | 0.48              |
| 1:b:123:ILE:HG23  | 1:b:191:LEU:HD13  | 1.94                     | 0.48              |
| 3:d:128:ALA:C     | 3:d:130:LYS:H     | 2.22                     | 0.48              |
| 5:f:82:PHE:CD2    | 5:f:137:LYS:HB2   | 2.48                     | 0.48              |
| 11:l:111:ILE:N    | 11:l:111:ILE:HD12 | 2.28                     | 0.48              |
| 13:n:45:ARG:HG3   | 13:n:95:THR:HG21  | 1.94                     | 0.48              |
| 35:K:47:LEU:HD21  | 35:K:57:ALA:HB3   | 1.94                     | 0.48              |
| 37:M:45:ILE:HD11  | 37:M:60:LEU:HA    | 1.95                     | 0.48              |
| 37:M:85:TYR:CD2   | 52:3:598:U:H4'    | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:X:17:LYS:NZ    | 48:X:31:ARG:O     | 2.46                     | 0.48              |
| 51:a:168:ASN:HD21 | 53:1:2179:C:H5'   | 1.79                     | 0.48              |
| 52:3:1170:A:H2'   | 52:3:1171:A:O4'   | 2.13                     | 0.48              |
| 53:1:457:A:O3'    | 53:1:458:G:H4'    | 2.12                     | 0.48              |
| 53:1:2713:U:H3'   | 53:1:2714:G:H5''  | 1.95                     | 0.48              |
| 53:1:2795:C:H2'   | 53:1:2796:U:O4'   | 2.13                     | 0.48              |
| 1:b:199:HIS:HE1   | 1:b:202:ARG:HH21  | 1.60                     | 0.48              |
| 1:b:217:PRO:HB3   | 53:1:1789:A:O3'   | 2.14                     | 0.48              |
| 2:c:16:THR:HG23   | 2:c:18:ASP:H      | 1.79                     | 0.48              |
| 31:G:107:ARG:O    | 31:G:110:ILE:HG22 | 2.13                     | 0.48              |
| 36:L:113:LYS:HB3  | 52:3:1297:G:H21   | 1.78                     | 0.48              |
| 37:M:72:GLU:HB2   | 37:M:129:ALA:O    | 2.14                     | 0.48              |
| 40:P:28:ASN:HB2   | 52:3:690:G:OP2    | 2.14                     | 0.48              |
| 42:R:77:LYS:NZ    | 53:1:888:C:H42    | 2.10                     | 0.48              |
| 44:T:57:ARG:HG2   | 44:T:57:ARG:HH11  | 1.78                     | 0.48              |
| 51:a:177:LYS:HZ3  | 53:1:2125:G:H5'   | 1.79                     | 0.48              |
| 52:3:1256:A:H1'   | 52:3:1258:G:N9    | 2.28                     | 0.48              |
| 53:1:861:A:H2'    | 53:1:862:G:O4'    | 2.14                     | 0.48              |
| 53:1:1299:G:O6    | 53:1:1639:C:H5''  | 2.13                     | 0.48              |
| 53:1:1827:U:O2'   | 53:1:1828:G:H5'   | 2.13                     | 0.48              |
| 5:f:131:VAL:HG13  | 5:f:131:VAL:O     | 2.14                     | 0.48              |
| 8:i:52:LEU:HD12   | 8:i:53:PRO:HD2    | 1.96                     | 0.48              |
| 32:H:4:VAL:O      | 32:H:6:PRO:HD3    | 2.14                     | 0.48              |
| 35:K:22:ILE:O     | 35:K:26:THR:HG22  | 2.13                     | 0.48              |
| 37:M:102:VAL:HG12 | 37:M:125:ILE:HD13 | 1.94                     | 0.48              |
| 43:S:80:ARG:HG3   | 43:S:81:ILE:HD12  | 1.95                     | 0.48              |
| 53:1:796:C:H2'    | 53:1:797:G:C8     | 2.48                     | 0.48              |
| 1:b:242:HIS:O     | 1:b:244:VAL:HG13  | 2.13                     | 0.48              |
| 3:d:41:GLN:HG3    | 3:d:43:THR:HG23   | 1.95                     | 0.48              |
| 6:g:22:LYS:HD2    | 53:1:2094:A:P     | 2.53                     | 0.48              |
| 7:h:56:ARG:HB2    | 53:1:1106:G:H4'   | 1.95                     | 0.48              |
| 7:h:118:ILE:N     | 7:h:119:PRO:HD2   | 2.29                     | 0.48              |
| 12:m:76:LYS:HB2   | 53:1:957:C:P      | 2.54                     | 0.48              |
| 18:s:97:LEU:HD12  | 18:s:97:LEU:N     | 2.29                     | 0.48              |
| 27:C:5:ARG:NH1    | 27:C:25:ASN:H     | 2.11                     | 0.48              |
| 33:I:14:GLU:OE1   | 33:I:59:LYS:HB3   | 2.14                     | 0.48              |
| 33:I:63:ILE:O     | 33:I:110:ARG:HD3  | 2.14                     | 0.48              |
| 38:N:70:GLY:HA3   | 52:3:1371:G:O3'   | 2.12                     | 0.48              |
| 38:N:74:GLN:O     | 38:N:78:ILE:HG13  | 2.13                     | 0.48              |
| 39:O:41:PRO:HG2   | 52:3:1150:A:C2    | 2.48                     | 0.48              |
| 46:V:13:SER:HB2   | 46:V:21:VAL:HG13  | 1.96                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 50:Z:66:ARG:HD2  | 52:3:1099:G:H4'   | 1.94                     | 0.48              |
| 1:b:32:LEU:HD23  | 1:b:102:TYR:HD2   | 1.79                     | 0.48              |
| 3:d:5:LEU:HD22   | 3:d:8:ALA:HB3     | 1.94                     | 0.48              |
| 3:d:52:VAL:O     | 3:d:54:GLY:N      | 2.46                     | 0.48              |
| 6:g:122:LEU:HD13 | 6:g:128:HIS:ND1   | 2.29                     | 0.48              |
| 10:k:24:VAL:HG11 | 10:k:30:ARG:HD3   | 1.95                     | 0.48              |
| 21:v:75:GLN:HB2  | 21:v:92:VAL:HG13  | 1.95                     | 0.48              |
| 26:B:4:GLN:O     | 53:1:2017:U:H4'   | 2.14                     | 0.48              |
| 31:G:130:LYS:HE2 | 52:3:1160:G:H5''  | 1.94                     | 0.48              |
| 52:3:1001:C:H2'  | 52:3:1002:G:H8    | 1.77                     | 0.48              |
| 54:2:3:C:H3'     | 54:2:4:C:C5'      | 2.43                     | 0.48              |
| 12:m:42:THR:HA   | 12:m:93:VAL:HA    | 1.94                     | 0.48              |
| 22:w:22:PHE:CD2  | 53:1:922:C:H1'    | 2.49                     | 0.48              |
| 25:z:15:ARG:N    | 25:z:15:ARG:HD2   | 2.29                     | 0.48              |
| 41:Q:74:GLN:HG2  | 41:Q:74:GLN:O     | 2.13                     | 0.48              |
| 51:a:175:ILE:HB  | 51:a:188:ASN:HB3  | 1.96                     | 0.48              |
| 53:1:873:C:H2'   | 53:1:874:G:C8     | 2.48                     | 0.48              |
| 53:1:2297:A:N6   | 53:1:2319:G:H1'   | 2.29                     | 0.48              |
| 53:1:2514:U:H2'  | 53:1:2515:C:C6    | 2.48                     | 0.48              |
| 53:1:2771:C:H2'  | 53:1:2772:C:C6    | 2.48                     | 0.48              |
| 54:2:63:C:H2'    | 54:2:64:G:H8      | 1.79                     | 0.48              |
| 1:b:164:VAL:CG1  | 52:3:712:A:H5''   | 2.43                     | 0.48              |
| 3:d:79:ARG:NH2   | 53:1:471:A:OP1    | 2.47                     | 0.48              |
| 6:g:116:ARG:O    | 6:g:118:PRO:HD3   | 2.14                     | 0.48              |
| 20:u:6:ARG:NH2   | 53:1:98:G:H1      | 2.10                     | 0.48              |
| 31:G:116:LEU:HG  | 31:G:140:LEU:HD13 | 1.96                     | 0.48              |
| 39:O:59:LYS:HE3  | 39:O:62:ARG:NH2   | 2.28                     | 0.48              |
| 48:X:76:THR:HG21 | 52:3:1221:G:O3'   | 2.14                     | 0.48              |
| 52:3:346:G:C2'   | 52:3:347:G:H5'    | 2.44                     | 0.48              |
| 53:1:327:G:H2'   | 53:1:328:U:O4'    | 2.13                     | 0.48              |
| 53:1:792:A:H3'   | 53:1:793:A:H5'    | 1.95                     | 0.48              |
| 53:1:1077:A:C3'  | 53:1:1078:U:H5'   | 2.43                     | 0.48              |
| 53:1:1330:C:H2'  | 53:1:1331:G:C8    | 2.49                     | 0.48              |
| 1:b:35:LYS:HB3   | 53:1:1570:A:H5'   | 1.96                     | 0.48              |
| 1:b:204:LEU:HB3  | 1:b:209:ALA:HB3   | 1.96                     | 0.48              |
| 3:d:130:LYS:HE3  | 3:d:132:LYS:HB3   | 1.95                     | 0.48              |
| 12:m:12:MET:HE3  | 12:m:71:LYS:HE3   | 1.95                     | 0.48              |
| 14:o:46:GLU:OE1  | 54:2:113:C:H4'    | 2.14                     | 0.48              |
| 18:s:18:ARG:HH12 | 53:1:518:G:P      | 2.37                     | 0.48              |
| 32:H:134:LYS:HA  | 32:H:137:VAL:HG22 | 1.96                     | 0.48              |
| 41:Q:100:ALA:H   | 41:Q:103:CYS:HB3  | 1.78                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 43:S:81:ILE:HG21 | 52:3:1202:U:H3    | 1.79                     | 0.48              |
| 48:X:9:PHE:CE1   | 52:3:1318:A:H4'   | 2.48                     | 0.48              |
| 52:3:1001:C:H2'  | 52:3:1002:G:C8    | 2.49                     | 0.48              |
| 53:1:704:G:H1'   | 53:1:727:A:H61    | 1.79                     | 0.48              |
| 53:1:2243:U:H2'  | 53:1:2244:U:C6    | 2.49                     | 0.48              |
| 1:b:97:ASP:HB3   | 53:1:1490:A:N7    | 2.27                     | 0.47              |
| 3:d:163:ASN:OD1  | 53:1:323:C:H5''   | 2.13                     | 0.47              |
| 16:q:86:SER:HB3  | 17:r:50:GLY:O     | 2.14                     | 0.47              |
| 24:y:41:HIS:CD2  | 53:1:96:C:H4'     | 2.48                     | 0.47              |
| 33:l:2:ARG:HH22  | 52:3:407:U:H5''   | 1.79                     | 0.47              |
| 36:L:148:LYS:HG2 | 36:L:148:LYS:O    | 2.13                     | 0.47              |
| 49:Y:41:GLY:HA2  | 49:Y:85:LEU:HD11  | 1.95                     | 0.47              |
| 52:3:558:G:H2'   | 52:3:559:A:C2     | 2.47                     | 0.47              |
| 53:1:1611:C:H6   | 53:1:1611:C:H5'   | 1.79                     | 0.47              |
| 53:1:1709:U:H2'  | 53:1:1710:G:C8    | 2.49                     | 0.47              |
| 53:1:2743:U:H2'  | 53:1:2744:G:O4'   | 2.13                     | 0.47              |
| 53:1:2743:U:C3'  | 53:1:2744:G:H5''  | 2.44                     | 0.47              |
| 1:b:159:THR:HG22 | 1:b:160:TYR:H     | 1.78                     | 0.47              |
| 10:k:35:VAL:HG13 | 10:k:36:GLY:N     | 2.28                     | 0.47              |
| 11:l:93:ASN:OD1  | 11:l:94:THR:HG23  | 2.14                     | 0.47              |
| 15:p:38:ARG:HD2  | 52:3:345:C:H5'    | 1.95                     | 0.47              |
| 15:p:112:ARG:C   | 15:p:113:LEU:HD23 | 2.39                     | 0.47              |
| 18:s:42:LYS:HB2  | 53:1:2010:G:H5''  | 1.95                     | 0.47              |
| 22:w:61:GLY:HA2  | 22:w:81:GLU:HB2   | 1.96                     | 0.47              |
| 27:C:35:LEU:HD21 | 53:1:2344:U:O2'   | 2.15                     | 0.47              |
| 34:J:25:LYS:HG2  | 52:3:923:A:OP1    | 2.13                     | 0.47              |
| 34:J:27:GLY:HA2  | 52:3:1398:A:H61   | 1.78                     | 0.47              |
| 36:L:113:LYS:NZ  | 52:3:1297:G:H1'   | 2.29                     | 0.47              |
| 42:R:27:THR:HG21 | 52:3:1328:C:H5''  | 1.95                     | 0.47              |
| 52:3:1273:C:H2'  | 52:3:1274:A:O4'   | 2.15                     | 0.47              |
| 53:1:1053:C:C3'  | 53:1:1054:A:H5''  | 2.43                     | 0.47              |
| 53:1:1720:U:H2'  | 53:1:1721:G:O4'   | 2.14                     | 0.47              |
| 53:1:2475:C:C2'  | 53:1:2476:A:H5'   | 2.44                     | 0.47              |
| 53:1:2515:C:H2'  | 53:1:2516:A:C8    | 2.49                     | 0.47              |
| 54:2:114:C:H2'   | 54:2:115:A:C8     | 2.49                     | 0.47              |
| 1:b:58:LYS:HE3   | 1:b:58:LYS:HB2    | 1.76                     | 0.47              |
| 1:b:175:LEU:HD13 | 53:1:1799:G:C8    | 2.49                     | 0.47              |
| 4:e:70:ARG:HH21  | 4:e:70:ARG:HG2    | 1.79                     | 0.47              |
| 18:s:42:LYS:HB3  | 53:1:2010:G:H5''  | 1.97                     | 0.47              |
| 31:G:40:ILE:H    | 31:G:40:ILE:HD12  | 1.80                     | 0.47              |
| 32:H:128:MET:HG3 | 32:H:131:ARG:HE   | 1.80                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 35:K:18:VAL:HB   | 35:K:19:PRO:HD3  | 1.95                     | 0.47              |
| 40:P:119:GLY:HA2 | 52:3:716:A:N3    | 2.29                     | 0.47              |
| 42:R:1:ALA:H1    | 42:R:52:ILE:HD13 | 1.79                     | 0.47              |
| 42:R:98:GLY:HA3  | 52:3:1322:C:H5'  | 1.96                     | 0.47              |
| 52:3:78:A:H2'    | 52:3:79:G:O4'    | 2.14                     | 0.47              |
| 52:3:335:C:H2'   | 52:3:336:A:H8    | 1.79                     | 0.47              |
| 52:3:346:G:H2'   | 52:3:347:G:H5'   | 1.96                     | 0.47              |
| 52:3:911:U:H2'   | 52:3:912:C:C6    | 2.49                     | 0.47              |
| 52:3:1352:C:H2'  | 52:3:1353:G:C8   | 2.48                     | 0.47              |
| 53:1:1306:C:H41  | 53:1:1606:C:H2'  | 1.79                     | 0.47              |
| 53:1:2029:G:O6   | 53:1:2032:G:H5'  | 2.13                     | 0.47              |
| 54:2:63:C:H2'    | 54:2:64:G:C8     | 2.49                     | 0.47              |
| 3:d:1:MET:O      | 3:d:14:VAL:HG12  | 2.13                     | 0.47              |
| 3:d:47:LYS:HE2   | 53:1:451:U:H4'   | 1.95                     | 0.47              |
| 4:e:69:ALA:HB2   | 4:e:84:ILE:HD12  | 1.96                     | 0.47              |
| 11:l:93:ASN:O    | 11:l:95:LEU:HD12 | 2.14                     | 0.47              |
| 29:E:61:LEU:HD12 | 29:E:61:LEU:O    | 2.14                     | 0.47              |
| 32:H:52:SER:HA   | 32:H:113:LYS:HG2 | 1.96                     | 0.47              |
| 40:P:96:ILE:HA   | 40:P:99:LEU:HD12 | 1.94                     | 0.47              |
| 45:U:38:PHE:CE1  | 45:U:51:ARG:HB2  | 2.49                     | 0.47              |
| 53:1:885:C:H2'   | 53:1:886:A:H8    | 1.80                     | 0.47              |
| 6:g:40:THR:HB    | 6:g:43:ASN:ND2   | 2.28                     | 0.47              |
| 32:H:38:VAL:O    | 32:H:42:LEU:HG   | 2.15                     | 0.47              |
| 33:I:7:LYS:HB3   | 33:I:20:LEU:HD23 | 1.96                     | 0.47              |
| 35:K:53:LYS:HG2  | 35:K:54:LEU:H    | 1.79                     | 0.47              |
| 38:N:60:LEU:HD12 | 38:N:60:LEU:O    | 2.15                     | 0.47              |
| 39:O:12:ALA:HB3  | 39:O:18:ILE:HG22 | 1.96                     | 0.47              |
| 52:3:946:A:H2'   | 52:3:947:G:H8    | 1.77                     | 0.47              |
| 52:3:1084:G:H2'  | 52:3:1085:U:C5   | 2.50                     | 0.47              |
| 53:1:2537:U:H2'  | 53:1:2538:C:C6   | 2.50                     | 0.47              |
| 54:2:28:C:H2'    | 54:2:29:A:H8     | 1.78                     | 0.47              |
| 6:g:12:LEU:HD12  | 6:g:13:GLY:N     | 2.30                     | 0.47              |
| 8:i:91:LYS:HB3   | 8:i:94:LYS:HE2   | 1.95                     | 0.47              |
| 10:k:5:GLN:N     | 10:k:21:CYS:O    | 2.43                     | 0.47              |
| 12:m:105:MET:HE2 | 12:m:117:PHE:CZ  | 2.49                     | 0.47              |
| 26:B:4:GLN:HB2   | 53:1:2054:A:C2   | 2.49                     | 0.47              |
| 33:I:112:GLU:O   | 33:I:115:GLN:HB3 | 2.15                     | 0.47              |
| 35:K:38:ARG:C    | 35:K:39:LEU:HD22 | 2.39                     | 0.47              |
| 36:L:37:THR:O    | 36:L:41:ILE:HG13 | 2.15                     | 0.47              |
| 40:P:50:GLY:HA2  | 40:P:52:ARG:NH1  | 2.29                     | 0.47              |
| 44:T:52:ARG:NH2  | 53:1:715:A:H61   | 2.12                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:T:74:VAL:HA    | 44:T:77:TYR:HB3   | 1.96                     | 0.47              |
| 51:a:8:MET:HG2    | 53:1:2175:C:OP1   | 2.14                     | 0.47              |
| 53:1:2038:G:H2'   | 53:1:2039:U:O4'   | 2.15                     | 0.47              |
| 53:1:2412:A:H2'   | 53:1:2413:G:O4'   | 2.14                     | 0.47              |
| 54:2:22:U:H2'     | 54:2:23:G:C8      | 2.49                     | 0.47              |
| 54:2:66:A:H5''    | 54:2:67:G:OP1     | 2.13                     | 0.47              |
| 2:c:52:THR:O      | 2:c:77:ARG:N      | 2.48                     | 0.47              |
| 2:c:73:VAL:HG22   | 2:c:74:GLU:N      | 2.30                     | 0.47              |
| 2:c:135:GLY:O     | 53:1:2580:U:H5''  | 2.15                     | 0.47              |
| 5:f:44:HIS:CG     | 5:f:45:ALA:H      | 2.31                     | 0.47              |
| 7:h:59:LEU:HB3    | 7:h:62:ARG:CB     | 2.45                     | 0.47              |
| 9:j:55:ILE:HD12   | 9:j:137:PRO:HG3   | 1.97                     | 0.47              |
| 10:k:18:ARG:HB2   | 10:k:45:GLU:HG3   | 1.97                     | 0.47              |
| 10:k:71:ARG:HH11  | 10:k:77:ILE:HD11  | 1.79                     | 0.47              |
| 11:l:29:LYS:HE3   | 53:1:566:U:H5''   | 1.97                     | 0.47              |
| 13:n:18:GLN:HE21  | 13:n:22:ARG:HH11  | 1.63                     | 0.47              |
| 15:p:112:ARG:O    | 15:p:113:LEU:HD23 | 2.15                     | 0.47              |
| 18:s:97:LEU:HD12  | 18:s:97:LEU:H     | 1.80                     | 0.47              |
| 31:G:22:TRP:HZ2   | 52:3:829:G:H4'    | 1.80                     | 0.47              |
| 33:I:187:ARG:HH22 | 33:I:192:ALA:HA   | 1.78                     | 0.47              |
| 36:L:91:ARG:O     | 36:L:95:ARG:N     | 2.48                     | 0.47              |
| 38:N:32:ARG:HD3   | 38:N:37:TYR:CE1   | 2.50                     | 0.47              |
| 40:P:53:GLY:H     | 40:P:56:LYS:HD3   | 1.79                     | 0.47              |
| 41:Q:30:ARG:HG2   | 52:3:363:A:OP2    | 2.15                     | 0.47              |
| 41:Q:119:LYS:HA   | 52:3:36:C:H4'     | 1.96                     | 0.47              |
| 42:R:76:ILE:O     | 42:R:80:MET:HG3   | 2.15                     | 0.47              |
| 43:S:1:ALA:HA     | 52:3:1203:C:OP1   | 2.14                     | 0.47              |
| 45:U:67:ILE:HG12  | 45:U:68:SER:N     | 2.30                     | 0.47              |
| 52:3:225:C:C3'    | 52:3:226:G:H5''   | 2.45                     | 0.47              |
| 52:3:505:G:OP2    | 52:3:534:U:H2'    | 2.15                     | 0.47              |
| 52:3:950:U:H2'    | 52:3:951:G:H8     | 1.78                     | 0.47              |
| 52:3:1016:A:H4'   | 52:3:1218:C:H4'   | 1.97                     | 0.47              |
| 52:3:1137:C:H4'   | 52:3:1138:G:N2    | 2.29                     | 0.47              |
| 52:3:1346:A:H2'   | 52:3:1347:G:H4'   | 1.97                     | 0.47              |
| 53:1:562:U:O4'    | 53:1:2036:C:H5'   | 2.15                     | 0.47              |
| 53:1:2001:C:H1'   | 53:1:2689:U:C4    | 2.50                     | 0.47              |
| 53:1:2529:G:H5''  | 53:1:2530:A:H5''  | 1.97                     | 0.47              |
| 53:1:2623:G:H2'   | 53:1:2624:G:C8    | 2.48                     | 0.47              |
| 55:5:57:A:H2'     | 55:5:58:A:C5'     | 2.39                     | 0.47              |
| 1:b:120:ASP:HB2   | 6:g:91:PHE:CE1    | 2.49                     | 0.47              |
| 1:b:209:ALA:HA    | 1:b:212:TRP:NE1   | 2.30                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 12:m:33:LEU:HB2   | 12:m:117:PHE:CD1 | 2.50                     | 0.47              |
| 27:C:11:VAL:HA    | 27:C:19:PHE:HB3  | 1.96                     | 0.47              |
| 29:E:39:ARG:HD2   | 53:1:2363:G:OP1  | 2.14                     | 0.47              |
| 32:H:102:ILE:HD12 | 32:H:102:ILE:H   | 1.78                     | 0.47              |
| 32:H:155:ARG:O    | 32:H:156:LEU:C   | 2.57                     | 0.47              |
| 43:S:30:ILE:HG22  | 43:S:30:ILE:O    | 2.15                     | 0.47              |
| 48:X:12:LEU:HG    | 48:X:16:LYS:HD2  | 1.97                     | 0.47              |
| 52:3:449:G:H2'    | 52:3:450:G:C8    | 2.50                     | 0.47              |
| 52:3:1033:G:C2'   | 52:3:1034:G:H5'' | 2.45                     | 0.47              |
| 53:1:581:C:H2'    | 53:1:582:A:H8    | 1.80                     | 0.47              |
| 53:1:942:G:H2'    | 53:1:943:A:O4'   | 2.14                     | 0.47              |
| 53:1:2366:A:H2'   | 53:1:2367:G:O4'  | 2.15                     | 0.47              |
| 53:1:2798:U:H4'   | 53:1:2799:A:C4   | 2.50                     | 0.47              |
| 1:b:47:ARG:HG2    | 53:1:773:U:O2'   | 2.15                     | 0.47              |
| 2:c:124:ARG:HD2   | 2:c:163:GLY:H    | 1.80                     | 0.47              |
| 3:d:30:GLN:O      | 3:d:33:VAL:HG12  | 2.15                     | 0.47              |
| 5:f:35:THR:C      | 5:f:36:LEU:HD22  | 2.40                     | 0.47              |
| 35:K:3:HIS:HB2    | 35:K:92:THR:CA   | 2.43                     | 0.47              |
| 40:P:24:ALA:HB1   | 40:P:89:GLY:HA3  | 1.96                     | 0.47              |
| 43:S:3:GLN:HE21   | 52:3:1047:G:H5'' | 1.80                     | 0.47              |
| 48:X:39:ILE:HB    | 48:X:66:VAL:HA   | 1.97                     | 0.47              |
| 51:a:45:ALA:HB3   | 51:a:213:SER:HB3 | 1.95                     | 0.47              |
| 52:3:358:U:H2'    | 52:3:359:G:C8    | 2.50                     | 0.47              |
| 52:3:1256:A:H1'   | 52:3:1258:G:C4   | 2.50                     | 0.47              |
| 53:1:395:U:H2'    | 53:1:396:G:C8    | 2.50                     | 0.47              |
| 53:1:534:U:H2'    | 53:1:535:G:C8    | 2.50                     | 0.47              |
| 53:1:1802:A:H2'   | 53:1:1803:A:C8   | 2.50                     | 0.47              |
| 53:1:2799:A:H2'   | 53:1:2800:A:H5'  | 1.96                     | 0.47              |
| 1:b:243:PRO:HG2   | 53:1:1901:A:O2'  | 2.14                     | 0.47              |
| 2:c:34:VAL:HA     | 2:c:50:VAL:HG12  | 1.96                     | 0.47              |
| 3:d:186:VAL:O     | 3:d:186:VAL:HG13 | 2.15                     | 0.47              |
| 7:h:59:LEU:HB3    | 7:h:62:ARG:HB2   | 1.96                     | 0.47              |
| 11:l:57:LEU:HD22  | 11:l:60:ARG:NH1  | 2.30                     | 0.47              |
| 22:w:51:ARG:NH1   | 53:1:2386:A:O3'  | 2.48                     | 0.47              |
| 26:B:54:ILE:HG23  | 26:B:56:LYS:H    | 1.80                     | 0.47              |
| 34:J:141:ASP:HA   | 34:J:144:GLU:HG2 | 1.96                     | 0.47              |
| 35:K:3:HIS:HA     | 35:K:65:GLU:HA   | 1.96                     | 0.47              |
| 53:1:1528:A:H2'   | 53:1:1529:G:O4'  | 2.15                     | 0.47              |
| 53:1:1600:C:H2'   | 53:1:1601:G:C8   | 2.50                     | 0.47              |
| 53:1:2605:U:H2'   | 53:1:2606:C:C6   | 2.50                     | 0.47              |
| 4:e:110:ILE:HG12  | 4:e:136:ILE:HG21 | 1.96                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:i:21:PRO:CB    | 8:i:22:PRO:HD3    | 2.46                     | 0.46              |
| 14:o:4:LYS:O     | 14:o:8:ILE:HG13   | 2.15                     | 0.46              |
| 14:o:52:SER:OG   | 14:o:54:VAL:HG12  | 2.15                     | 0.46              |
| 23:x:13:THR:CG2  | 53:1:188:G:H5'    | 2.45                     | 0.46              |
| 25:z:8:GLN:HA    | 25:z:54:VAL:HG12  | 1.97                     | 0.46              |
| 31:G:213:LEU:HA  | 31:G:216:VAL:HG22 | 1.96                     | 0.46              |
| 33:I:150:LYS:HB2 | 33:I:155:LYS:HD3  | 1.96                     | 0.46              |
| 34:J:28:ARG:NH1  | 52:3:15:G:H4'     | 2.28                     | 0.46              |
| 53:1:817:C:H2'   | 53:1:818:G:O4'    | 2.15                     | 0.46              |
| 53:1:974:G:N3    | 53:1:974:G:H2'    | 2.30                     | 0.46              |
| 53:1:2233:U:H2'  | 53:1:2234:G:C8    | 2.50                     | 0.46              |
| 53:1:2743:U:H3'  | 53:1:2744:G:H5''  | 1.97                     | 0.46              |
| 1:b:48:ILE:HG23  | 1:b:48:ILE:O      | 2.15                     | 0.46              |
| 3:d:122:GLU:HG3  | 3:d:123:LYS:H     | 1.80                     | 0.46              |
| 8:i:38:CYS:HA    | 8:i:41:PHE:HB3    | 1.98                     | 0.46              |
| 23:x:29:LEU:CD2  | 53:1:2230:G:H5''  | 2.44                     | 0.46              |
| 24:y:1:MET:O     | 24:y:5:GLU:HG2    | 2.15                     | 0.46              |
| 30:F:18:LYS:HD3  | 30:F:18:LYS:O     | 2.15                     | 0.46              |
| 31:G:162:VAL:HB  | 31:G:184:ALA:HB2  | 1.96                     | 0.46              |
| 33:I:25:ARG:HD3  | 33:I:28:ASP:HA    | 1.96                     | 0.46              |
| 43:S:52:ARG:HH12 | 48:X:36:ARG:NH2   | 2.13                     | 0.46              |
| 45:U:44:SER:H    | 45:U:46:LYS:NZ    | 2.13                     | 0.46              |
| 52:3:1420:U:O2'  | 52:3:1421:G:H5'   | 2.15                     | 0.46              |
| 53:1:27:G:N2     | 53:1:512:G:H1'    | 2.29                     | 0.46              |
| 53:1:343:C:O2'   | 53:1:344:A:H5'    | 2.14                     | 0.46              |
| 53:1:2676:C:H2'  | 53:1:2677:G:H8    | 1.79                     | 0.46              |
| 12:m:14:LYS:HB3  | 53:1:954:G:OP2    | 2.15                     | 0.46              |
| 12:m:93:VAL:HG12 | 12:m:94:ALA:N     | 2.30                     | 0.46              |
| 13:n:55:ALA:HA   | 13:n:80:PHE:CE1   | 2.50                     | 0.46              |
| 25:z:4:ILE:HD11  | 25:z:56:VAL:HG13  | 1.98                     | 0.46              |
| 32:H:10:ARG:HA   | 32:H:13:ILE:HD11  | 1.97                     | 0.46              |
| 33:I:78:ALA:HA   | 33:I:81:LEU:HD12  | 1.96                     | 0.46              |
| 40:P:27:ASN:O    | 40:P:56:LYS:HB3   | 2.15                     | 0.46              |
| 41:Q:11:ARG:HB3  | 52:3:562:U:O2'    | 2.16                     | 0.46              |
| 42:R:53:ASP:HA   | 42:R:56:ARG:HH11  | 1.80                     | 0.46              |
| 52:3:206:C:H2'   | 52:3:207:C:O4'    | 2.15                     | 0.46              |
| 53:1:326:G:H2'   | 53:1:327:G:H8     | 1.81                     | 0.46              |
| 53:1:438:G:H2'   | 53:1:439:A:C8     | 2.51                     | 0.46              |
| 53:1:1678:A:H2'  | 53:1:1679:A:O4'   | 2.15                     | 0.46              |
| 4:e:12:VAL:O     | 4:e:16:MET:HG2    | 2.15                     | 0.46              |
| 10:k:88:ASN:HB2  | 10:k:91:SER:O     | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:w:39:THR:HB    | 53:1:2331:G:O2'   | 2.15                     | 0.46              |
| 28:D:30:VAL:HG11  | 53:1:466:A:H4'    | 1.96                     | 0.46              |
| 34:J:101:GLY:H    | 34:J:121:ASN:HB3  | 1.80                     | 0.46              |
| 34:J:163:ILE:HD12 | 34:J:163:ILE:N    | 2.30                     | 0.46              |
| 35:K:18:VAL:HG21  | 35:K:58:HIS:CD2   | 2.50                     | 0.46              |
| 38:N:6:TYR:CE2    | 52:3:1147:C:H4'   | 2.51                     | 0.46              |
| 38:N:105:ARG:NH1  | 38:N:107:ALA:HA   | 2.29                     | 0.46              |
| 40:P:55:ARG:HH22  | 55:6:39:C:H4'     | 1.79                     | 0.46              |
| 42:R:72:ILE:O     | 42:R:76:ILE:HG13  | 2.15                     | 0.46              |
| 42:R:89:ARG:CZ    | 42:R:94:LEU:HB3   | 2.46                     | 0.46              |
| 50:Z:39:LYS:N     | 50:Z:40:PRO:CD    | 2.79                     | 0.46              |
| 52:3:717:U:H2'    | 52:3:734:G:OP2    | 2.16                     | 0.46              |
| 53:1:680:C:H2'    | 53:1:681:G:C8     | 2.49                     | 0.46              |
| 53:1:2019:A:H2    | 53:1:2035:G:H22   | 1.63                     | 0.46              |
| 53:1:2220:U:H2'   | 53:1:2221:G:H8    | 1.81                     | 0.46              |
| 3:d:14:VAL:HG22   | 3:d:15:SER:H      | 1.81                     | 0.46              |
| 3:d:36:ALA:HB1    | 53:1:443:A:H62    | 1.80                     | 0.46              |
| 7:h:28:ALA:HA     | 7:h:56:ARG:HH22   | 1.80                     | 0.46              |
| 7:h:97:LYS:HE3    | 7:h:125:ARG:HD2   | 1.97                     | 0.46              |
| 9:j:59:ALA:HB3    | 9:j:126:ALA:HA    | 1.97                     | 0.46              |
| 12:m:35:ALA:HA    | 12:m:128:THR:HG22 | 1.97                     | 0.46              |
| 12:m:53:MET:O     | 12:m:57:VAL:HG22  | 2.15                     | 0.46              |
| 12:m:77:PRO:HB2   | 12:m:80:VAL:HG21  | 1.97                     | 0.46              |
| 19:t:69:ARG:HH21  | 53:1:1335:C:P     | 2.39                     | 0.46              |
| 23:x:29:LEU:HD23  | 53:1:2230:G:H5''  | 1.97                     | 0.46              |
| 25:z:50:VAL:O     | 25:z:54:VAL:HG22  | 2.16                     | 0.46              |
| 35:K:93:LYS:HG2   | 35:K:93:LYS:O     | 2.16                     | 0.46              |
| 49:Y:28:ARG:HA    | 49:Y:31:ILE:HG22  | 1.97                     | 0.46              |
| 49:Y:59:ARG:HD3   | 52:3:177:G:OP2    | 2.15                     | 0.46              |
| 52:3:571:U:H4'    | 52:3:819:A:C6     | 2.51                     | 0.46              |
| 52:3:955:U:H2'    | 52:3:956:U:O4'    | 2.16                     | 0.46              |
| 53:1:248:G:H3'    | 53:1:249:C:C5'    | 2.46                     | 0.46              |
| 53:1:414:C:H2'    | 53:1:415:A:C8     | 2.51                     | 0.46              |
| 53:1:531:C:O2'    | 53:1:563:A:H5''   | 2.15                     | 0.46              |
| 53:1:660:C:H2'    | 53:1:661:A:C8     | 2.51                     | 0.46              |
| 53:1:1234:U:H2'   | 53:1:1235:G:O4'   | 2.15                     | 0.46              |
| 53:1:1373:A:C5'   | 53:1:2212:A:H1'   | 2.46                     | 0.46              |
| 54:2:51:G:H2'     | 54:2:52:A:O4'     | 2.15                     | 0.46              |
| 54:2:88:C:C4'     | 54:2:89:U:OP1     | 2.62                     | 0.46              |
| 4:e:134:GLN:HE22  | 4:e:149:ARG:H     | 1.63                     | 0.46              |
| 4:e:137:PHE:HB3   | 4:e:139:GLU:OE1   | 2.16                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:h:37:LYS:HE2    | 53:1:1085:A:H62  | 1.79                     | 0.46              |
| 12:m:40:ARG:HH12  | 12:m:73:ILE:HG21 | 1.80                     | 0.46              |
| 16:q:65:ASN:ND2   | 16:q:69:ARG:HE   | 2.09                     | 0.46              |
| 20:u:50:ALA:O     | 20:u:51:LEU:HB3  | 2.16                     | 0.46              |
| 22:w:51:ARG:C     | 22:w:51:ARG:HD3  | 2.40                     | 0.46              |
| 31:G:8:MET:HE2    | 31:G:13:VAL:HG11 | 1.98                     | 0.46              |
| 42:R:85:TYR:O     | 42:R:88:LEU:HG   | 2.16                     | 0.46              |
| 45:U:12:LYS:HG2   | 52:3:44:A:P      | 2.55                     | 0.46              |
| 52:3:1458:G:H2'   | 52:3:1459:G:C8   | 2.51                     | 0.46              |
| 53:1:251:A:H2'    | 53:1:252:G:O4'   | 2.16                     | 0.46              |
| 54:2:65:U:O4      | 54:2:108:A:H2'   | 2.16                     | 0.46              |
| 1:b:68:ARG:NH1    | 1:b:128:THR:OG1  | 2.49                     | 0.46              |
| 16:q:66:ALA:O     | 16:q:70:GLN:HG2  | 2.16                     | 0.46              |
| 19:t:39:THR:O     | 19:t:43:ILE:HG13 | 2.15                     | 0.46              |
| 19:t:80:TRP:CZ3   | 19:t:82:LYS:HB3  | 2.51                     | 0.46              |
| 28:D:1:MET:HE1    | 53:1:789:A:H2    | 1.80                     | 0.46              |
| 32:H:87:ARG:HH21  | 32:H:88:LYS:HZ1  | 1.63                     | 0.46              |
| 32:H:181:ILE:HG13 | 32:H:202:PHE:HA  | 1.98                     | 0.46              |
| 33:I:199:ILE:O    | 33:I:202:LEU:HG  | 2.16                     | 0.46              |
| 42:R:78:ARG:NH1   | 42:R:79:LEU:HD21 | 2.30                     | 0.46              |
| 53:1:69:C:H2'     | 53:1:70:G:C8     | 2.51                     | 0.46              |
| 53:1:123:G:H2'    | 53:1:124:G:O4'   | 2.16                     | 0.46              |
| 53:1:253:C:H2'    | 53:1:254:G:O4'   | 2.16                     | 0.46              |
| 53:1:1313:U:H2'   | 53:1:1610:A:C2   | 2.51                     | 0.46              |
| 4:e:135:ILE:HG21  | 4:e:142:TYR:CD1  | 2.51                     | 0.46              |
| 8:i:15:GLY:HA3    | 8:i:51:GLY:H     | 1.79                     | 0.46              |
| 9:j:18:VAL:HG23   | 9:j:54:ILE:HD11  | 1.98                     | 0.46              |
| 14:o:25:ARG:HD2   | 14:o:93:ASP:OD1  | 2.16                     | 0.46              |
| 15:p:92:ARG:HD3   | 53:1:1753:G:H5'' | 1.98                     | 0.46              |
| 17:r:76:LYS:HE2   | 53:1:992:C:OP1   | 2.16                     | 0.46              |
| 33:I:147:LYS:HE3  | 52:3:490:C:H5''  | 1.98                     | 0.46              |
| 37:M:28:SER:HB3   | 37:M:58:LEU:HB2  | 1.98                     | 0.46              |
| 48:X:28:LYS:NZ    | 48:X:31:ARG:HD2  | 2.31                     | 0.46              |
| 52:3:193:C:H2'    | 52:3:194:C:C6    | 2.51                     | 0.46              |
| 52:3:1219:A:H2'   | 52:3:1220:G:C8   | 2.51                     | 0.46              |
| 52:3:1374:A:H2'   | 52:3:1375:A:O4'  | 2.16                     | 0.46              |
| 53:1:255:A:H2'    | 53:1:256:A:O4'   | 2.15                     | 0.46              |
| 53:1:611:C:H2'    | 53:1:612:G:O4'   | 2.16                     | 0.46              |
| 53:1:1023:U:H4'   | 53:1:1123:C:OP1  | 2.14                     | 0.46              |
| 53:1:1432:G:H2'   | 53:1:1433:A:C8   | 2.51                     | 0.46              |
| 3:d:97:ASN:HB2    | 3:d:100:MET:CG   | 2.46                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:h:53:ARG:HG2    | 7:h:55:VAL:HG23  | 1.98                     | 0.46              |
| 8:i:135:MET:HE1   | 53:1:1062:G:N3   | 2.30                     | 0.46              |
| 11:l:79:LEU:O     | 11:l:82:LEU:HD23 | 2.16                     | 0.46              |
| 15:p:1:SER:HB2    | 15:p:3:ILE:HD13  | 1.97                     | 0.46              |
| 27:C:32:LYS:HA    | 27:C:50:GLU:OE2  | 2.16                     | 0.46              |
| 29:E:36:ALA:H     | 29:E:39:ARG:HD3  | 1.80                     | 0.46              |
| 35:K:3:HIS:HD2    | 35:K:92:THR:HB   | 1.80                     | 0.46              |
| 36:L:109:LYS:HG3  | 36:L:110:ARG:N   | 2.29                     | 0.46              |
| 38:N:32:ARG:HD3   | 38:N:37:TYR:CD1  | 2.50                     | 0.46              |
| 40:P:125:LYS:HD2  | 52:3:797:C:OP2   | 2.16                     | 0.46              |
| 53:1:184:C:H2'    | 53:1:185:G:H8    | 1.81                     | 0.46              |
| 53:1:239:C:H2'    | 53:1:240:C:O4'   | 2.16                     | 0.46              |
| 53:1:479:A:H1'    | 53:1:481:G:H5''  | 1.98                     | 0.46              |
| 53:1:1367:A:C2'   | 53:1:1368:G:H5'  | 2.46                     | 0.46              |
| 53:1:2197:U:O2'   | 53:1:2198:A:H5'' | 2.16                     | 0.46              |
| 53:1:2834:G:O2'   | 53:1:2835:A:H5'  | 2.16                     | 0.46              |
| 57:7:61:C:H5'     | 57:7:61:C:H6     | 1.81                     | 0.46              |
| 8:i:29:GLN:HG3    | 8:i:30:GLN:NE2   | 2.31                     | 0.46              |
| 11:l:63:LYS:CB    | 29:E:12:ARG:HG2  | 2.45                     | 0.46              |
| 11:l:93:ASN:C     | 11:l:95:LEU:H    | 2.23                     | 0.46              |
| 13:n:44:LEU:O     | 13:n:48:VAL:HG12 | 2.16                     | 0.46              |
| 20:u:45:GLN:O     | 20:u:55:GLY:HA2  | 2.15                     | 0.46              |
| 22:w:51:ARG:HD3   | 22:w:51:ARG:O    | 2.16                     | 0.46              |
| 28:D:13:ASN:O     | 53:1:125:A:H4'   | 2.16                     | 0.46              |
| 37:M:50:VAL:HG22  | 37:M:50:VAL:O    | 2.16                     | 0.46              |
| 37:M:124:ILE:HG23 | 37:M:124:ILE:O   | 2.16                     | 0.46              |
| 42:R:24:VAL:HG23  | 42:R:28:ARG:HG3  | 1.98                     | 0.46              |
| 43:S:15:LEU:HD12  | 43:S:18:LYS:HE2  | 1.97                     | 0.46              |
| 52:3:291:U:H2'    | 52:3:292:G:C8    | 2.51                     | 0.46              |
| 52:3:867:G:H2'    | 52:3:868:C:C6    | 2.51                     | 0.46              |
| 53:1:1625:C:H2'   | 53:1:1626:A:O4'  | 2.17                     | 0.46              |
| 53:1:2545:G:H2'   | 53:1:2546:U:O4'  | 2.16                     | 0.46              |
| 53:1:2663:G:H2'   | 53:1:2664:G:O4'  | 2.16                     | 0.46              |
| 1:b:30:ALA:HB3    | 1:b:31:PRO:HD3   | 1.97                     | 0.45              |
| 1:b:216:ARG:NH2   | 53:1:781:A:OP1   | 2.49                     | 0.45              |
| 8:i:58:ILE:HD12   | 8:i:58:ILE:N     | 2.31                     | 0.45              |
| 9:j:84:ILE:HG23   | 9:j:84:ILE:O     | 2.15                     | 0.45              |
| 10:k:6:THR:HG23   | 53:1:1666:G:O3'  | 2.16                     | 0.45              |
| 10:k:102:PRO:HG3  | 15:p:69:VAL:HG22 | 1.98                     | 0.45              |
| 12:m:74:THR:HG22  | 12:m:89:VAL:HG22 | 1.96                     | 0.45              |
| 13:n:38:LEU:HB3   | 13:n:39:PRO:HD3  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 20:u:93:ARG:HB2  | 20:u:102:ILE:HD12 | 1.98                     | 0.45              |
| 21:v:30:ILE:HD12 | 21:v:91:PHE:O     | 2.16                     | 0.45              |
| 28:D:11:LYS:HE3  | 53:1:686:U:C4'    | 2.46                     | 0.45              |
| 33:I:77:GLU:O    | 33:I:81:LEU:HG    | 2.17                     | 0.45              |
| 35:K:35:LYS:O    | 35:K:64:VAL:HG23  | 2.15                     | 0.45              |
| 39:O:59:LYS:HD2  | 52:3:972:C:O3'    | 2.17                     | 0.45              |
| 40:P:12:ARG:HB3  | 40:P:75:GLU:HB3   | 1.99                     | 0.45              |
| 41:Q:20:VAL:C    | 41:Q:22:ALA:H     | 2.24                     | 0.45              |
| 52:3:981:U:H2'   | 52:3:982:U:C5     | 2.51                     | 0.45              |
| 52:3:1404:C:H2'  | 52:3:1405:G:C8    | 2.51                     | 0.45              |
| 52:3:1486:G:H2'  | 52:3:1487:G:C8    | 2.51                     | 0.45              |
| 53:1:340:A:H2'   | 53:1:341:C:O4'    | 2.16                     | 0.45              |
| 53:1:1130:U:O2'  | 53:1:1131:G:OP1   | 2.30                     | 0.45              |
| 53:1:1258:U:H2'  | 53:1:1259:G:C8    | 2.51                     | 0.45              |
| 53:1:1936:A:H3'  | 53:1:1937:A:H5'   | 1.98                     | 0.45              |
| 53:1:2487:G:H2'  | 53:1:2488:G:C8    | 2.52                     | 0.45              |
| 11:l:38:GLN:HB3  | 53:1:832:U:C5'    | 2.41                     | 0.45              |
| 11:l:77:ILE:CD1  | 11:l:108:ALA:HB1  | 2.46                     | 0.45              |
| 12:m:33:LEU:HD13 | 12:m:117:PHE:HB3  | 1.98                     | 0.45              |
| 17:r:90:ARG:NH2  | 53:1:1222:U:OP2   | 2.49                     | 0.45              |
| 19:t:6:ARG:HG2   | 19:t:6:ARG:HH11   | 1.80                     | 0.45              |
| 19:t:18:GLU:O    | 19:t:22:THR:HG23  | 2.15                     | 0.45              |
| 19:t:93:LEU:HD23 | 19:t:93:LEU:O     | 2.16                     | 0.45              |
| 31:G:40:ILE:HD12 | 31:G:40:ILE:N     | 2.31                     | 0.45              |
| 37:M:93:LYS:O    | 37:M:93:LYS:HD2   | 2.16                     | 0.45              |
| 39:O:15:HIS:HA   | 39:O:18:ILE:HG12  | 1.98                     | 0.45              |
| 41:Q:113:ARG:HB2 | 41:Q:118:VAL:O    | 2.16                     | 0.45              |
| 51:a:39:VAL:HG13 | 51:a:39:VAL:O     | 2.16                     | 0.45              |
| 52:3:757:U:H2'   | 52:3:758:C:O4'    | 2.17                     | 0.45              |
| 52:3:1464:U:H2'  | 52:3:1465:A:C8    | 2.52                     | 0.45              |
| 53:1:794:A:H2'   | 53:1:795:C:O4'    | 2.16                     | 0.45              |
| 53:1:2292:U:H2'  | 53:1:2293:G:C8    | 2.51                     | 0.45              |
| 57:7:68:C:H2'    | 57:7:69:G:C8      | 2.52                     | 0.45              |
| 1:b:159:THR:HG22 | 1:b:160:TYR:N     | 2.31                     | 0.45              |
| 8:i:14:ALA:HB2   | 8:i:54:ILE:HB     | 1.98                     | 0.45              |
| 12:m:42:THR:CG2  | 12:m:45:GLN:HG3   | 2.46                     | 0.45              |
| 18:s:84:ARG:HE   | 53:1:1323:C:H5''  | 1.81                     | 0.45              |
| 22:w:51:ARG:CZ   | 53:1:2386:A:H5''  | 2.47                     | 0.45              |
| 23:x:31:ASN:HD22 | 23:x:52:ALA:HB2   | 1.81                     | 0.45              |
| 23:x:36:ARG:HG3  | 23:x:47:THR:HB    | 1.98                     | 0.45              |
| 26:B:30:ASP:HB3  | 26:B:34:GLY:N     | 2.30                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:E:23:HIS:HD2   | 29:E:49:VAL:HG12  | 1.82                     | 0.45              |
| 32:H:176:THR:HB   | 32:H:179:ALA:HB2  | 1.97                     | 0.45              |
| 36:L:15:PRO:HB2   | 38:N:44:ARG:NH1   | 2.31                     | 0.45              |
| 36:L:49:LEU:HD12  | 36:L:50:ALA:N     | 2.30                     | 0.45              |
| 48:X:35:ARG:CZ    | 48:X:74:ALA:HB3   | 2.46                     | 0.45              |
| 49:Y:34:VAL:O     | 49:Y:38:ILE:HG13  | 2.15                     | 0.45              |
| 52:3:79:G:O2'     | 52:3:80:A:H5'     | 2.16                     | 0.45              |
| 52:3:1391:U:H2'   | 52:3:1392:G:H8    | 1.82                     | 0.45              |
| 53:1:244:A:H62    | 53:1:254:G:H21    | 1.63                     | 0.45              |
| 53:1:319:G:H2'    | 53:1:320:A:O4'    | 2.16                     | 0.45              |
| 53:1:607:U:O4     | 53:1:620:G:H5'    | 2.17                     | 0.45              |
| 53:1:2800:A:H3'   | 53:1:2801:G:H5'   | 1.98                     | 0.45              |
| 54:2:108:A:H5'    | 54:2:109:A:O5'    | 2.16                     | 0.45              |
| 4:e:12:VAL:HG13   | 4:e:13:LYS:N      | 2.31                     | 0.45              |
| 4:e:73:VAL:HG12   | 4:e:78:ILE:HG12   | 1.99                     | 0.45              |
| 4:e:125:GLY:HA2   | 4:e:162:ASP:HA    | 1.99                     | 0.45              |
| 6:g:80:ILE:HD12   | 6:g:80:ILE:N      | 2.32                     | 0.45              |
| 6:g:135:HIS:HB3   | 6:g:138:VAL:HB    | 1.98                     | 0.45              |
| 7:h:56:ARG:CZ     | 7:h:83:ALA:HB2    | 2.46                     | 0.45              |
| 8:i:9:LYS:HD3     | 53:1:1061:U:OP1   | 2.16                     | 0.45              |
| 12:m:105:MET:HE2  | 12:m:117:PHE:CE2  | 2.51                     | 0.45              |
| 20:u:10:VAL:HG22  | 20:u:11:ILE:N     | 2.32                     | 0.45              |
| 38:N:117:LEU:HD22 | 38:N:117:LEU:N    | 2.32                     | 0.45              |
| 45:U:80:LYS:N     | 45:U:80:LYS:HD3   | 2.31                     | 0.45              |
| 49:Y:70:LYS:HD3   | 52:3:262:A:OP2    | 2.15                     | 0.45              |
| 52:3:423:G:H2'    | 52:3:424:G:H5'    | 1.98                     | 0.45              |
| 52:3:1449:C:H2'   | 52:3:1450:U:O4'   | 2.15                     | 0.45              |
| 53:1:613:A:H2'    | 53:1:613:A:N3     | 2.32                     | 0.45              |
| 53:1:2039:U:H2'   | 53:1:2040:G:C8    | 2.51                     | 0.45              |
| 53:1:2051:A:H2'   | 53:1:2578:G:OP1   | 2.16                     | 0.45              |
| 53:1:2215:C:H2'   | 53:1:2216:G:C8    | 2.51                     | 0.45              |
| 53:1:2710:C:H2'   | 53:1:2711:A:C8    | 2.52                     | 0.45              |
| 54:2:97:C:H2'     | 54:2:98:G:O4'     | 2.15                     | 0.45              |
| 55:6:28:C:H2'     | 55:6:29:G:C8      | 2.51                     | 0.45              |
| 2:c:181:ASP:OD1   | 2:c:184:ARG:HG2   | 2.17                     | 0.45              |
| 3:d:1:MET:N       | 3:d:14:VAL:O      | 2.50                     | 0.45              |
| 5:f:67:ALA:HA     | 5:f:70:LEU:HD12   | 1.97                     | 0.45              |
| 8:i:79:LEU:HD21   | 8:i:105:LEU:HD21  | 1.99                     | 0.45              |
| 13:n:79:LEU:O     | 13:n:80:PHE:HB2   | 2.16                     | 0.45              |
| 31:G:119:GLN:O    | 31:G:124:THR:HG22 | 2.17                     | 0.45              |
| 34:J:25:LYS:HG2   | 52:3:922:G:O3'    | 2.15                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:N:122:ARG:NH1  | 52:3:1350:A:OP1   | 2.50                     | 0.45              |
| 40:P:81:LEU:C     | 40:P:81:LEU:HD12  | 2.42                     | 0.45              |
| 41:Q:23:LEU:HB3   | 41:Q:26:CYS:SG    | 2.57                     | 0.45              |
| 46:V:58:VAL:HG22  | 46:V:74:LEU:HD11  | 1.99                     | 0.45              |
| 52:3:1435:G:H2'   | 52:3:1436:U:C6    | 2.51                     | 0.45              |
| 53:1:1417:C:H4'   | 53:1:1587:G:H21   | 1.81                     | 0.45              |
| 53:1:2452:C:H42   | 53:1:2504:U:H3    | 1.65                     | 0.45              |
| 3:d:63:LYS:HD2    | 53:1:2444:G:P     | 2.57                     | 0.45              |
| 4:e:147:ARG:HG3   | 4:e:149:ARG:NH2   | 2.32                     | 0.45              |
| 13:n:98:LEU:HD11  | 13:n:114:GLU:OE2  | 2.17                     | 0.45              |
| 15:p:109:ILE:HG22 | 15:p:110:LYS:H    | 1.82                     | 0.45              |
| 29:E:29:ARG:HG3   | 53:1:2394:C:OP2   | 2.16                     | 0.45              |
| 33:I:78:ALA:HB1   | 33:I:85:THR:HG23  | 1.98                     | 0.45              |
| 33:I:100:VAL:HG21 | 33:I:136:VAL:HG21 | 1.99                     | 0.45              |
| 35:K:14:GLN:HG2   | 35:K:83:ALA:HB2   | 1.99                     | 0.45              |
| 35:K:51:ILE:C     | 35:K:53:LYS:H     | 2.25                     | 0.45              |
| 36:L:2:ARG:HG3    | 52:3:932:C:OP2    | 2.16                     | 0.45              |
| 49:Y:79:THR:O     | 49:Y:83:ASN:ND2   | 2.50                     | 0.45              |
| 51:a:46:VAL:HG22  | 51:a:212:VAL:HG13 | 1.99                     | 0.45              |
| 52:3:396:C:H3'    | 52:3:397:A:H5''   | 1.99                     | 0.45              |
| 53:1:11:C:H3'     | 53:1:12:U:C5'     | 2.46                     | 0.45              |
| 53:1:249:C:H2'    | 53:1:2394:C:O2'   | 2.15                     | 0.45              |
| 53:1:1093:G:H21   | 53:1:1098:A:H62   | 1.65                     | 0.45              |
| 53:1:1796:U:H2'   | 53:1:1797:G:C8    | 2.48                     | 0.45              |
| 53:1:1987:A:H2'   | 53:1:1988:G:C8    | 2.52                     | 0.45              |
| 53:1:2219:U:H2'   | 53:1:2220:U:O4'   | 2.17                     | 0.45              |
| 1:b:212:TRP:HE1   | 1:b:213:ARG:NH1   | 2.15                     | 0.45              |
| 16:q:44:TYR:O     | 16:q:47:ARG:HG2   | 2.16                     | 0.45              |
| 16:q:61:ILE:HG21  | 53:1:1009:A:C4'   | 2.37                     | 0.45              |
| 22:w:73:ARG:NH2   | 53:1:2332:C:H5''  | 2.31                     | 0.45              |
| 30:F:1:MET:HE2    | 30:F:34:LYS:HZ2   | 1.82                     | 0.45              |
| 31:G:187:ASP:HB3  | 31:G:189:ASN:OD1  | 2.17                     | 0.45              |
| 37:M:3:GLN:HE22   | 52:3:755:G:N2     | 2.14                     | 0.45              |
| 37:M:17:GLN:HG2   | 37:M:62:LEU:HD23  | 1.98                     | 0.45              |
| 45:U:12:LYS:HE2   | 45:U:12:LYS:HA    | 1.99                     | 0.45              |
| 46:V:48:GLU:HB2   | 46:V:51:GLU:OE1   | 2.16                     | 0.45              |
| 48:X:24:SER:OG    | 48:X:27:LYS:HD3   | 2.15                     | 0.45              |
| 53:1:1275:A:N6    | 53:1:1296:G:H4'   | 2.32                     | 0.45              |
| 53:1:2633:G:H5''  | 53:1:2812:G:H5'   | 1.98                     | 0.45              |
| 8:i:93:ASN:HD21   | 53:1:1077:A:H4'   | 1.81                     | 0.45              |
| 14:o:16:ARG:O     | 14:o:19:GLN:HG2   | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:s:31:GLN:O     | 18:s:35:ILE:HG13  | 2.17                     | 0.45              |
| 26:B:15:ARG:NH1   | 53:1:1264:A:OP1   | 2.50                     | 0.45              |
| 32:H:175:HIS:ND1  | 52:3:1109:C:OP2   | 2.50                     | 0.45              |
| 51:a:170:ILE:HD12 | 51:a:170:ILE:N    | 2.32                     | 0.45              |
| 52:3:225:C:C2'    | 52:3:226:G:H5''   | 2.47                     | 0.45              |
| 52:3:1481:U:H2'   | 52:3:1482:G:C8    | 2.52                     | 0.45              |
| 53:1:732:C:H2'    | 53:1:733:G:O4'    | 2.16                     | 0.45              |
| 53:1:1679:A:H2'   | 53:1:1680:U:C6    | 2.51                     | 0.45              |
| 53:1:2177:C:H2'   | 53:1:2178:C:O4'   | 2.17                     | 0.45              |
| 1:b:224:MET:HE2   | 53:1:782:A:C6     | 2.52                     | 0.45              |
| 3:d:15:SER:HB3    | 3:d:18:THR:HG22   | 1.99                     | 0.45              |
| 3:d:127:GLU:HG2   | 3:d:128:ALA:N     | 2.32                     | 0.45              |
| 12:m:10:ARG:NE    | 53:1:2278:A:OP1   | 2.49                     | 0.45              |
| 15:p:57:ALA:HA    | 15:p:75:THR:HG23  | 1.99                     | 0.45              |
| 16:q:22:GLY:HA2   | 53:1:19:A:H5'     | 1.98                     | 0.45              |
| 16:q:89:ILE:HD11  | 17:r:40:MET:HE2   | 1.98                     | 0.45              |
| 19:t:61:LEU:HD13  | 53:1:1340:U:C2'   | 2.42                     | 0.45              |
| 20:u:4:ILE:HD12   | 20:u:4:ILE:H      | 1.81                     | 0.45              |
| 20:u:52:ASN:CG    | 20:u:54:PRO:HD3   | 2.41                     | 0.45              |
| 21:v:49:ASN:HD21  | 53:1:1040:A:H5'   | 1.79                     | 0.45              |
| 24:y:19:LEU:O     | 24:y:23:ARG:NE    | 2.49                     | 0.45              |
| 33:I:134:TYR:HE1  | 52:3:620:C:H5'    | 1.81                     | 0.45              |
| 37:M:9:MET:HA     | 37:M:26:MET:HE1   | 1.99                     | 0.45              |
| 42:R:74:MET:SD    | 42:R:74:MET:C     | 3.00                     | 0.45              |
| 42:R:90:HIS:CE1   | 42:R:108:ARG:HH22 | 2.34                     | 0.45              |
| 45:U:67:ILE:HG12  | 45:U:68:SER:H     | 1.82                     | 0.45              |
| 45:U:76:LYS:O     | 45:U:79:ASN:HB2   | 2.17                     | 0.45              |
| 47:W:28:LEU:HG    | 47:W:67:LEU:HD11  | 1.99                     | 0.45              |
| 47:W:40:PRO:HB3   | 52:3:720:C:H5''   | 1.99                     | 0.45              |
| 49:Y:53:MET:SD    | 49:Y:54:GLN:N     | 2.89                     | 0.45              |
| 52:3:620:C:H2'    | 52:3:621:A:O4'    | 2.16                     | 0.45              |
| 52:3:1346:A:C2'   | 52:3:1347:G:H4'   | 2.46                     | 0.45              |
| 53:1:12:U:O2'     | 53:1:13:A:H5'     | 2.16                     | 0.45              |
| 53:1:87:U:H5''    | 53:1:88:G:H5'     | 1.98                     | 0.45              |
| 53:1:975:A:H1'    | 53:1:990:A:N1     | 2.32                     | 0.45              |
| 53:1:1019:U:H2'   | 53:1:1020:A:C8    | 2.51                     | 0.45              |
| 53:1:1590:A:H2'   | 53:1:1591:A:C8    | 2.52                     | 0.45              |
| 53:1:2062:A:H4'   | 53:1:2442:C:OP2   | 2.17                     | 0.45              |
| 53:1:2215:C:H2'   | 53:1:2216:G:H8    | 1.82                     | 0.45              |
| 7:h:118:ILE:O     | 7:h:118:ILE:HG22  | 2.17                     | 0.45              |
| 8:i:16:MET:HE1    | 8:i:19:PRO:HB3    | 1.98                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:j:37:ARG:NE    | 9:j:44:TYR:OH     | 2.49                     | 0.45              |
| 10:k:63:VAL:HG23 | 10:k:107:LEU:HD11 | 1.99                     | 0.45              |
| 18:s:71:VAL:HG13 | 18:s:71:VAL:O     | 2.16                     | 0.45              |
| 35:K:26:THR:O    | 35:K:29:ILE:HG22  | 2.17                     | 0.45              |
| 35:K:75:GLU:HA   | 35:K:78:PHE:CD2   | 2.51                     | 0.45              |
| 35:K:77:THR:HB   | 35:K:81:ASN:HD21  | 1.82                     | 0.45              |
| 39:O:42:LEU:HD22 | 39:O:71:LEU:HD22  | 1.99                     | 0.45              |
| 43:S:30:ILE:HD12 | 43:S:30:ILE:N     | 2.32                     | 0.45              |
| 50:Z:25:ALA:HB1  | 50:Z:29:ALA:HB2   | 1.98                     | 0.45              |
| 52:3:163:C:H2'   | 52:3:164:G:O4'    | 2.16                     | 0.45              |
| 52:3:598:U:H2'   | 52:3:599:C:C6     | 2.51                     | 0.45              |
| 52:3:966:G:C2    | 55:5:34:C:H5'     | 2.52                     | 0.45              |
| 53:1:145:C:H2'   | 53:1:146:A:C8     | 2.52                     | 0.45              |
| 53:1:176:A:O2'   | 53:1:177:G:H5'    | 2.16                     | 0.45              |
| 53:1:471:A:H2'   | 53:1:472:A:O4'    | 2.17                     | 0.45              |
| 53:1:542:C:C2'   | 53:1:543:G:H5''   | 2.45                     | 0.45              |
| 53:1:1054:A:H2'  | 53:1:1055:G:C8    | 2.51                     | 0.45              |
| 53:1:1444:G:H2'  | 53:1:1445:G:C8    | 2.52                     | 0.45              |
| 53:1:2644:G:H3'  | 53:1:2645:G:N2    | 2.32                     | 0.45              |
| 53:1:2743:U:H2'  | 53:1:2744:G:H5''  | 1.99                     | 0.45              |
| 53:1:2853:C:H2'  | 53:1:2854:G:C8    | 2.52                     | 0.45              |
| 55:6:11:A:H2'    | 55:6:12:G:C8      | 2.52                     | 0.45              |
| 6:g:15:LEU:HD21  | 6:g:56:ALA:HB1    | 1.98                     | 0.44              |
| 6:g:100:ALA:HA   | 6:g:103:VAL:HG12  | 1.98                     | 0.44              |
| 9:j:77:HIS:HA    | 9:j:84:ILE:HA     | 1.99                     | 0.44              |
| 11:l:23:ILE:HG12 | 17:r:82:HIS:NE2   | 2.32                     | 0.44              |
| 12:m:14:LYS:HE3  | 53:1:956:G:O6     | 2.17                     | 0.44              |
| 15:p:13:LYS:HE3  | 15:p:76:HIS:HA    | 1.99                     | 0.44              |
| 22:w:74:LYS:HD2  | 22:w:74:LYS:N     | 2.32                     | 0.44              |
| 24:y:39:GLN:HB3  | 24:y:41:HIS:CE1   | 2.52                     | 0.44              |
| 32:H:51:VAL:HA   | 32:H:69:THR:HA    | 1.99                     | 0.44              |
| 32:H:160:GLU:H   | 32:H:160:GLU:CD   | 2.24                     | 0.44              |
| 43:S:14:ALA:O    | 43:S:17:ASP:OD2   | 2.35                     | 0.44              |
| 44:T:32:THR:O    | 44:T:35:ILE:HG12  | 2.16                     | 0.44              |
| 53:1:2220:U:H2'  | 53:1:2221:G:C8    | 2.52                     | 0.44              |
| 2:c:14:ILE:HB    | 2:c:22:ILE:HB     | 1.99                     | 0.44              |
| 2:c:168:GLU:HG2  | 2:c:169:ARG:N     | 2.32                     | 0.44              |
| 4:e:132:ARG:O    | 4:e:148:VAL:HG12  | 2.17                     | 0.44              |
| 12:m:76:LYS:HG3  | 53:1:956:G:H5''   | 1.98                     | 0.44              |
| 14:o:7:ARG:HA    | 14:o:10:ARG:HH11  | 1.82                     | 0.44              |
| 28:D:35:ARG:HE   | 53:1:54:G:H1'     | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:H:161:ILE:HG22 | 32:H:163:ARG:HH21 | 1.81                     | 0.44              |
| 33:I:193:ASP:OD2  | 33:I:194:ILE:HD12 | 2.17                     | 0.44              |
| 36:L:55:LYS:HB3   | 36:L:59:GLU:HG2   | 1.99                     | 0.44              |
| 37:M:101:ALA:HB1  | 37:M:124:ILE:HD11 | 2.00                     | 0.44              |
| 41:Q:43:LYS:HZ1   | 56:4:20:U:C3'     | 2.30                     | 0.44              |
| 43:S:15:LEU:CD2   | 43:S:53:ASP:HB3   | 2.45                     | 0.44              |
| 52:3:219:U:H2'    | 52:3:220:G:C8     | 2.52                     | 0.44              |
| 53:1:2248:C:C2'   | 53:1:2249:U:H5'   | 2.47                     | 0.44              |
| 1:b:131:MET:HG3   | 1:b:187:CYS:O     | 2.17                     | 0.44              |
| 5:f:157:LYS:HD2   | 53:1:2659:G:OP1   | 2.17                     | 0.44              |
| 12:m:93:VAL:HG12  | 12:m:94:ALA:H     | 1.82                     | 0.44              |
| 16:q:58:GLN:HA    | 16:q:61:ILE:HB    | 1.99                     | 0.44              |
| 16:q:61:ILE:HD11  | 16:q:75:TYR:CZ    | 2.53                     | 0.44              |
| 21:v:7:GLU:O      | 21:v:41:GLU:HB3   | 2.17                     | 0.44              |
| 22:w:73:ARG:HH22  | 53:1:2333:A:P     | 2.41                     | 0.44              |
| 32:H:161:ILE:HG22 | 32:H:163:ARG:NH2  | 2.33                     | 0.44              |
| 37:M:83:ARG:HH21  | 52:3:644:U:C5'    | 2.30                     | 0.44              |
| 41:Q:79:ILE:HD12  | 41:Q:96:THR:OG1   | 2.16                     | 0.44              |
| 45:U:21:VAL:HG13  | 45:U:21:VAL:O     | 2.17                     | 0.44              |
| 49:Y:66:ILE:C     | 49:Y:68:LYS:H     | 2.25                     | 0.44              |
| 52:3:784:A:H2'    | 52:3:785:G:C8     | 2.52                     | 0.44              |
| 52:3:1453:G:H3'   | 52:3:1453:G:N3    | 2.32                     | 0.44              |
| 53:1:278:A:H2'    | 53:1:278:A:N3     | 2.33                     | 0.44              |
| 53:1:1153:C:H2'   | 53:1:1154:G:O4'   | 2.16                     | 0.44              |
| 4:e:65:LEU:HD12   | 54:2:42:C:N4      | 2.32                     | 0.44              |
| 6:g:75:LEU:HD12   | 6:g:76:GLU:N      | 2.32                     | 0.44              |
| 23:x:16:ASN:HD22  | 23:x:16:ASN:HA    | 1.50                     | 0.44              |
| 24:y:23:ARG:O     | 24:y:25:GLN:N     | 2.50                     | 0.44              |
| 27:C:33:LEU:HD12  | 27:C:33:LEU:H     | 1.82                     | 0.44              |
| 28:D:34:ARG:NH2   | 28:D:41:ARG:O     | 2.51                     | 0.44              |
| 32:H:27:GLU:OE1   | 32:H:27:GLU:N     | 2.45                     | 0.44              |
| 33:I:58:GLN:OE1   | 33:I:61:ARG:NE    | 2.47                     | 0.44              |
| 42:R:102:LYS:HG3  | 52:3:1226:C:N4    | 2.32                     | 0.44              |
| 45:U:76:LYS:HE2   | 52:3:474:G:OP1    | 2.17                     | 0.44              |
| 52:3:5:U:H4'      | 52:3:6:G:C8       | 2.53                     | 0.44              |
| 52:3:1225:A:H2'   | 52:3:1225:A:N3    | 2.33                     | 0.44              |
| 52:3:1236:A:H4'   | 52:3:1304:G:H4'   | 1.98                     | 0.44              |
| 53:1:1322:A:N6    | 53:1:1333:G:H21   | 2.14                     | 0.44              |
| 53:1:1736:U:H2'   | 53:1:1737:G:O4'   | 2.18                     | 0.44              |
| 53:1:2233:U:H2'   | 53:1:2234:G:H8    | 1.83                     | 0.44              |
| 53:1:2326:C:O2'   | 53:1:2327:A:OP1   | 2.31                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 54:2:88:C:H5''   | 54:2:89:U:OP1     | 2.17                     | 0.44              |
| 3:d:102:ARG:HE   | 3:d:200:LEU:HA    | 1.82                     | 0.44              |
| 6:g:62:LEU:HD23  | 6:g:62:LEU:O      | 2.17                     | 0.44              |
| 15:p:29:VAL:HG23 | 15:p:79:VAL:HG12  | 2.00                     | 0.44              |
| 21:v:19:ARG:NH2  | 54:2:95:U:OP2     | 2.50                     | 0.44              |
| 26:B:17:SER:HB3  | 53:1:15:G:H4'     | 2.00                     | 0.44              |
| 29:E:39:ARG:HG2  | 53:1:2363:G:OP2   | 2.18                     | 0.44              |
| 33:I:145:ARG:NH1 | 52:3:490:C:OP1    | 2.50                     | 0.44              |
| 34:J:25:LYS:HG2  | 52:3:923:A:P      | 2.57                     | 0.44              |
| 38:N:34:LEU:HD23 | 38:N:34:LEU:N     | 2.33                     | 0.44              |
| 41:Q:122:LYS:N   | 41:Q:122:LYS:CD   | 2.78                     | 0.44              |
| 42:R:79:LEU:HB3  | 42:R:84:CYS:SG    | 2.58                     | 0.44              |
| 46:V:11:VAL:HG11 | 46:V:20:ILE:HD11  | 2.00                     | 0.44              |
| 46:V:18:LYS:CE   | 52:3:255:G:H4'    | 2.47                     | 0.44              |
| 49:Y:67:HIS:CE1  | 52:3:132:C:H4'    | 2.51                     | 0.44              |
| 51:a:174:THR:CB  | 53:1:2124:G:H5''  | 2.42                     | 0.44              |
| 52:3:784:A:H4'   | 53:1:1837:C:OP1   | 2.17                     | 0.44              |
| 52:3:1258:G:H2'  | 52:3:1259:C:C6    | 2.52                     | 0.44              |
| 53:1:548:G:H2'   | 53:1:549:G:O4'    | 2.17                     | 0.44              |
| 53:1:1201:U:H2'  | 53:1:1202:G:C8    | 2.52                     | 0.44              |
| 53:1:2487:G:H2'  | 53:1:2488:G:H8    | 1.83                     | 0.44              |
| 53:1:2698:U:H2'  | 53:1:2699:C:C6    | 2.53                     | 0.44              |
| 3:d:3:LEU:HB3    | 3:d:120:VAL:HG21  | 2.00                     | 0.44              |
| 3:d:97:ASN:HB2   | 3:d:100:MET:HG3   | 1.99                     | 0.44              |
| 12:m:36:VAL:HG21 | 12:m:129:THR:HG23 | 1.98                     | 0.44              |
| 25:z:46:MET:HE2  | 53:1:851:C:H1'    | 2.00                     | 0.44              |
| 32:H:171:ARG:C   | 32:H:173:PRO:HD3  | 2.42                     | 0.44              |
| 33:I:166:LYS:N   | 33:I:167:PRO:HD3  | 2.31                     | 0.44              |
| 47:W:53:GLN:HA   | 47:W:56:ARG:HE    | 1.83                     | 0.44              |
| 53:1:20:C:H2'    | 53:1:21:A:H8      | 1.82                     | 0.44              |
| 53:1:123:G:O2'   | 53:1:1376:C:H4'   | 2.16                     | 0.44              |
| 53:1:832:U:H2'   | 53:1:833:A:C8     | 2.53                     | 0.44              |
| 53:1:905:A:O2'   | 53:1:906:U:H5'    | 2.17                     | 0.44              |
| 53:1:1947:C:H2'  | 53:1:1948:G:C8    | 2.53                     | 0.44              |
| 53:1:2221:G:O2'  | 53:1:2222:C:H5'   | 2.17                     | 0.44              |
| 53:1:2743:U:H2'  | 53:1:2744:G:C4'   | 2.47                     | 0.44              |
| 4:e:17:THR:O     | 4:e:20:ASN:ND2    | 2.50                     | 0.44              |
| 5:f:82:PHE:CZ    | 5:f:137:LYS:HE3   | 2.52                     | 0.44              |
| 6:g:43:ASN:HA    | 6:g:46:PHE:CD2    | 2.53                     | 0.44              |
| 6:g:73:ASN:HB3   | 6:g:108:VAL:HG23  | 1.99                     | 0.44              |
| 7:h:56:ARG:HE    | 7:h:81:LEU:HG     | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:k:31:ARG:H    | 10:k:31:ARG:HD2  | 1.81                     | 0.44              |
| 12:m:86:LYS:NZ   | 53:1:955:U:H5''  | 2.33                     | 0.44              |
| 14:o:34:HIS:CE1  | 14:o:65:THR:HG21 | 2.53                     | 0.44              |
| 25:z:6:ILE:HD13  | 25:z:56:VAL:HG22 | 2.00                     | 0.44              |
| 31:G:140:LEU:O   | 31:G:144:GLU:HG2 | 2.18                     | 0.44              |
| 34:J:125:LYS:HD3 | 52:3:8:A:H5''    | 2.00                     | 0.44              |
| 35:K:54:LEU:HD23 | 35:K:54:LEU:H    | 1.82                     | 0.44              |
| 35:K:81:ASN:O    | 35:K:84:VAL:HG22 | 2.17                     | 0.44              |
| 36:L:31:VAL:HG22 | 36:L:32:ASP:N    | 2.33                     | 0.44              |
| 37:M:80:PRO:HG2  | 52:3:878:A:C5'   | 2.48                     | 0.44              |
| 38:N:27:ILE:HB   | 38:N:34:LEU:HD13 | 2.00                     | 0.44              |
| 45:U:38:PHE:CZ   | 45:U:51:ARG:HB2  | 2.52                     | 0.44              |
| 49:Y:49:ALA:HA   | 49:Y:52:GLU:HB2  | 2.00                     | 0.44              |
| 50:Z:28:LEU:H    | 50:Z:28:LEU:HD12 | 1.82                     | 0.44              |
| 52:3:539:A:H2'   | 52:3:540:G:C8    | 2.52                     | 0.44              |
| 52:3:674:G:H2'   | 52:3:675:A:C8    | 2.52                     | 0.44              |
| 52:3:889:A:O3'   | 52:3:890:G:H4'   | 2.18                     | 0.44              |
| 52:3:1458:G:H2'  | 52:3:1459:G:H8   | 1.83                     | 0.44              |
| 53:1:362:A:H3'   | 53:1:363:G:H8    | 1.83                     | 0.44              |
| 53:1:634:C:H2'   | 53:1:635:C:C6    | 2.51                     | 0.44              |
| 53:1:1434:A:H2'  | 53:1:1435:G:C8   | 2.53                     | 0.44              |
| 53:1:1967:C:H2'  | 53:1:1968:G:O4'  | 2.18                     | 0.44              |
| 53:1:2087:G:H2'  | 53:1:2088:A:C8   | 2.52                     | 0.44              |
| 53:1:2224:G:H4'  | 53:1:2226:C:O2   | 2.18                     | 0.44              |
| 2:c:173:GLN:HB2  | 53:1:2731:G:H5'  | 1.99                     | 0.44              |
| 14:o:40:ILE:HD13 | 54:2:8:C:O2'     | 2.18                     | 0.44              |
| 14:o:75:GLY:O    | 14:o:78:VAL:HG22 | 2.17                     | 0.44              |
| 17:r:63:VAL:HA   | 17:r:96:VAL:HA   | 2.00                     | 0.44              |
| 31:G:44:LYS:HA   | 31:G:44:LYS:HD3  | 1.88                     | 0.44              |
| 36:L:63:VAL:HA   | 36:L:66:GLU:HG2  | 1.99                     | 0.44              |
| 37:M:38:VAL:O    | 37:M:41:GLU:HG3  | 2.17                     | 0.44              |
| 38:N:94:ARG:HA   | 38:N:97:LEU:HB3  | 2.00                     | 0.44              |
| 48:X:55:GLN:HG2  | 48:X:56:HIS:N    | 2.33                     | 0.44              |
| 51:a:69:THR:HA   | 51:a:176:GLY:HA2 | 2.00                     | 0.44              |
| 52:3:1004:A:H2'  | 52:3:1005:A:O4'  | 2.18                     | 0.44              |
| 52:3:1305:G:H22  | 52:3:1331:G:H2'  | 1.83                     | 0.44              |
| 53:1:755:U:H2'   | 53:1:756:A:C8    | 2.52                     | 0.44              |
| 53:1:881:G:O2'   | 53:1:882:G:H5'   | 2.18                     | 0.44              |
| 53:1:1680:U:C2'  | 53:1:1681:G:H5'  | 2.48                     | 0.44              |
| 1:b:77:VAL:HG23  | 1:b:77:VAL:O     | 2.17                     | 0.44              |
| 2:c:142:VAL:HG22 | 2:c:143:PRO:HD2  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:d:131:THR:HG23 | 53:1:321:U:H5''   | 2.00                     | 0.44              |
| 7:h:33:VAL:HG12  | 7:h:34:THR:N      | 2.31                     | 0.44              |
| 8:i:23:VAL:HG12  | 8:i:26:ALA:HB3    | 1.99                     | 0.44              |
| 9:j:66:GLY:HA3   | 53:1:1141:U:C5    | 2.52                     | 0.44              |
| 12:m:12:MET:HG3  | 12:m:72:PRO:HG2   | 2.00                     | 0.44              |
| 16:q:23:TYR:O    | 53:1:18:U:H5''    | 2.18                     | 0.44              |
| 20:u:56:GLY:N    | 53:1:483:A:O2'    | 2.50                     | 0.44              |
| 25:z:29:ARG:CD   | 53:1:1183:U:H5''  | 2.48                     | 0.44              |
| 31:G:205:ALA:O   | 31:G:209:VAL:HG23 | 2.18                     | 0.44              |
| 42:R:3:ILE:O     | 42:R:4:ALA:C      | 2.61                     | 0.44              |
| 44:T:23:SER:O    | 44:T:27:GLN:HG3   | 2.18                     | 0.44              |
| 50:Z:44:ARG:NH1  | 52:3:722:G:OP2    | 2.51                     | 0.44              |
| 53:1:703:U:H2'   | 53:1:704:G:O4'    | 2.18                     | 0.44              |
| 53:1:967:U:H2'   | 53:1:968:C:C6     | 2.53                     | 0.44              |
| 1:b:229:HIS:ND1  | 1:b:230:PRO:HD2   | 2.33                     | 0.43              |
| 14:o:51:ALA:HB2  | 14:o:81:ARG:HD2   | 2.00                     | 0.43              |
| 26:B:8:THR:HG21  | 53:1:2021:C:OP1   | 2.17                     | 0.43              |
| 28:D:21:ARG:O    | 28:D:27:GLY:HA3   | 2.18                     | 0.43              |
| 31:G:27:LYS:HB3  | 31:G:28:PRO:HD3   | 2.00                     | 0.43              |
| 32:H:4:VAL:HB    | 52:3:1190:G:P     | 2.58                     | 0.43              |
| 33:I:18:LEU:HB2  | 33:I:20:LEU:HD13  | 2.00                     | 0.43              |
| 34:J:75:LEU:O    | 34:J:75:LEU:HD12  | 2.18                     | 0.43              |
| 35:K:66:ALA:HB1  | 35:K:67:PRO:HD2   | 1.99                     | 0.43              |
| 37:M:83:ARG:HH21 | 52:3:644:U:C4'    | 2.31                     | 0.43              |
| 44:T:44:GLU:C    | 44:T:46:LYS:H     | 2.26                     | 0.43              |
| 46:V:27:PHE:CD1  | 46:V:38:LYS:HE2   | 2.53                     | 0.43              |
| 52:3:37:U:H3     | 52:3:397:A:H61    | 1.66                     | 0.43              |
| 52:3:256:U:H2'   | 52:3:257:G:C8     | 2.53                     | 0.43              |
| 52:3:1501:C:H5'' | 52:3:1502:A:OP2   | 2.18                     | 0.43              |
| 53:1:274:C:H2'   | 53:1:275:C:O4'    | 2.18                     | 0.43              |
| 53:1:1083:U:H2'  | 53:1:1085:A:OP2   | 2.18                     | 0.43              |
| 53:1:1219:U:H2'  | 53:1:1220:G:C8    | 2.53                     | 0.43              |
| 53:1:1935:G:O2'  | 53:1:1936:A:H5'   | 2.18                     | 0.43              |
| 53:1:2004:G:H2'  | 53:1:2005:A:O4'   | 2.18                     | 0.43              |
| 53:1:2293:G:H2'  | 53:1:2294:G:C8    | 2.53                     | 0.43              |
| 54:2:60:C:H2'    | 54:2:61:G:H8      | 1.83                     | 0.43              |
| 5:f:34:ARG:HA    | 5:f:34:ARG:HD2    | 1.84                     | 0.43              |
| 9:j:74:TYR:OH    | 9:j:100:VAL:HG13  | 2.18                     | 0.43              |
| 12:m:36:VAL:HG23 | 12:m:128:THR:HA   | 1.99                     | 0.43              |
| 20:u:42:LYS:HE3  | 53:1:499:U:H5''   | 1.99                     | 0.43              |
| 21:v:82:TYR:HE2  | 21:v:83:LYS:HZ3   | 1.63                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 29:E:44:ARG:NH2   | 53:1:2418:A:OP1  | 2.50                     | 0.43              |
| 34:J:108:GLY:O    | 34:J:109:ALA:HB3 | 2.18                     | 0.43              |
| 38:N:66:VAL:HG22  | 38:N:67:LYS:N    | 2.33                     | 0.43              |
| 46:V:58:VAL:HG22  | 46:V:59:GLU:H    | 1.83                     | 0.43              |
| 51:a:23:ILE:HG12  | 51:a:186:LYS:HE2 | 1.99                     | 0.43              |
| 52:3:76:G:H2'     | 52:3:77:A:O4'    | 2.18                     | 0.43              |
| 53:1:685:A:H1'    | 53:1:688:U:O4    | 2.18                     | 0.43              |
| 53:1:1071:G:OP1   | 53:1:1071:G:H3'  | 2.18                     | 0.43              |
| 53:1:2572:A:OP1   | 53:1:2574:G:H4'  | 2.18                     | 0.43              |
| 54:2:35:C:C2'     | 54:2:36:C:H5'    | 2.48                     | 0.43              |
| 5:f:25:ILE:HG22   | 5:f:78:VAL:HG11  | 2.00                     | 0.43              |
| 13:n:18:GLN:HE21  | 13:n:22:ARG:NH1  | 2.17                     | 0.43              |
| 14:o:33:ARG:HB2   | 54:2:52:A:H62    | 1.81                     | 0.43              |
| 23:x:39:VAL:HG11  | 23:x:42:GLU:HB2  | 2.01                     | 0.43              |
| 29:E:44:ARG:N     | 29:E:45:PRO:HD2  | 2.33                     | 0.43              |
| 31:G:20:ARG:HG3   | 52:3:830:G:O2'   | 2.18                     | 0.43              |
| 32:H:124:GLU:C    | 32:H:125:ARG:HD2 | 2.43                     | 0.43              |
| 33:I:8:LEU:HD11   | 33:I:21:LYS:HB2  | 2.01                     | 0.43              |
| 34:J:24:VAL:HG13  | 34:J:26:GLY:H    | 1.82                     | 0.43              |
| 40:P:111:ASP:HB3  | 50:Z:3:ILE:HA    | 2.01                     | 0.43              |
| 43:S:26:LEU:HD21  | 43:S:46:LYS:HD3  | 1.99                     | 0.43              |
| 44:T:3:SER:O      | 44:T:7:THR:HG23  | 2.17                     | 0.43              |
| 51:a:222:VAL:HG13 | 51:a:222:VAL:O   | 2.18                     | 0.43              |
| 53:1:1278:C:H2'   | 53:1:1279:G:C8   | 2.53                     | 0.43              |
| 53:1:1487:U:H2'   | 53:1:1488:C:C6   | 2.53                     | 0.43              |
| 53:1:2580:U:H2'   | 53:1:2581:G:H5'  | 2.00                     | 0.43              |
| 53:1:2819:G:H2'   | 53:1:2821:A:N7   | 2.33                     | 0.43              |
| 2:c:8:LYS:HB2     | 2:c:201:LEU:HD12 | 2.00                     | 0.43              |
| 7:h:58:THR:HG21   | 7:h:82:ILE:H     | 1.83                     | 0.43              |
| 10:k:29:HIS:O     | 10:k:31:ARG:HD2  | 2.18                     | 0.43              |
| 13:n:39:PRO:HG2   | 53:1:1651:G:H4'  | 1.98                     | 0.43              |
| 16:q:4:LYS:HE3    | 53:1:30:G:OP1    | 2.17                     | 0.43              |
| 25:z:2:LYS:HG3    | 25:z:39:ASP:HB3  | 2.00                     | 0.43              |
| 28:D:35:ARG:HH21  | 53:1:54:G:H1'    | 1.83                     | 0.43              |
| 32:H:45:GLU:HG2   | 32:H:86:LEU:HD11 | 2.00                     | 0.43              |
| 39:O:6:ILE:HD12   | 39:O:6:ILE:N     | 2.34                     | 0.43              |
| 40:P:121:ARG:HA   | 40:P:122:PRO:HD3 | 1.79                     | 0.43              |
| 42:R:77:LYS:NZ    | 53:1:888:C:N3    | 2.64                     | 0.43              |
| 45:U:6:LEU:HD22   | 45:U:17:TYR:HB3  | 1.99                     | 0.43              |
| 52:3:211:G:C2'    | 52:3:212:G:H5'   | 2.48                     | 0.43              |
| 52:3:791:G:N2     | 52:3:1497:G:H4'  | 2.33                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 52:3:1397:C:H42   | 56:4:22:A:H2'    | 1.82                     | 0.43              |
| 53:1:403:U:O3'    | 53:1:404:A:H4'   | 2.19                     | 0.43              |
| 53:1:948:C:H2'    | 53:1:949:G:C8    | 2.54                     | 0.43              |
| 53:1:1078:U:C5'   | 53:1:1079:C:H5'' | 2.47                     | 0.43              |
| 53:1:1182:G:H2'   | 53:1:1183:U:O4'  | 2.19                     | 0.43              |
| 53:1:2011:U:H2'   | 53:1:2012:G:O4'  | 2.19                     | 0.43              |
| 53:1:2197:U:H1'   | 53:1:2198:A:C8   | 2.53                     | 0.43              |
| 54:2:66:A:H4'     | 54:2:67:G:C8     | 2.54                     | 0.43              |
| 3:d:122:GLU:HG3   | 3:d:123:LYS:N    | 2.33                     | 0.43              |
| 7:h:73:LYS:HD2    | 7:h:76:PHE:HD2   | 1.82                     | 0.43              |
| 8:i:23:VAL:CG1    | 8:i:26:ALA:HB3   | 2.47                     | 0.43              |
| 9:j:73:VAL:O      | 9:j:73:VAL:HG13  | 2.18                     | 0.43              |
| 14:o:71:ALA:HB2   | 14:o:102:ARG:HG2 | 1.99                     | 0.43              |
| 15:p:101:GLU:HG3  | 15:p:102:ARG:HG3 | 2.00                     | 0.43              |
| 19:t:32:LEU:HD23  | 19:t:32:LEU:H    | 1.82                     | 0.43              |
| 30:F:36:ARG:O     | 30:F:37:GLN:O    | 2.37                     | 0.43              |
| 33:I:33:ILE:HG12  | 33:I:34:GLU:N    | 2.34                     | 0.43              |
| 33:I:131:ILE:HD13 | 52:3:620:C:C1'   | 2.49                     | 0.43              |
| 38:N:83:THR:HG22  | 38:N:97:LEU:HD11 | 2.01                     | 0.43              |
| 43:S:74:ARG:HG2   | 43:S:74:ARG:HH11 | 1.83                     | 0.43              |
| 44:T:47:LYS:HE3   | 52:3:808:C:OP2   | 2.18                     | 0.43              |
| 52:3:67:C:H2'     | 52:3:68:G:C8     | 2.53                     | 0.43              |
| 52:3:392:C:H2'    | 52:3:393:A:C8    | 2.54                     | 0.43              |
| 52:3:467:U:H5'    | 52:3:468:A:OP2   | 2.19                     | 0.43              |
| 53:1:1360:G:H22   | 53:1:2214:C:H42  | 1.65                     | 0.43              |
| 53:1:2128:G:H21   | 53:1:2173:A:H1'  | 1.83                     | 0.43              |
| 53:1:2368:C:H2'   | 53:1:2369:A:H8   | 1.83                     | 0.43              |
| 57:7:70:G:H2'     | 57:7:71:G:O4'    | 2.17                     | 0.43              |
| 1:b:23:LEU:HD23   | 1:b:24:HIS:O     | 2.18                     | 0.43              |
| 5:f:75:VAL:O      | 5:f:79:THR:HG22  | 2.18                     | 0.43              |
| 5:f:97:VAL:HG12   | 5:f:124:CYS:SG   | 2.58                     | 0.43              |
| 18:s:8:ARG:HD2    | 53:1:494:G:OP1   | 2.19                     | 0.43              |
| 45:U:36:VAL:HG13  | 45:U:36:VAL:O    | 2.18                     | 0.43              |
| 52:3:166:U:H2'    | 52:3:167:A:C8    | 2.53                     | 0.43              |
| 52:3:434:U:H2'    | 52:3:435:A:C8    | 2.53                     | 0.43              |
| 53:1:69:C:O2'     | 53:1:70:G:H5'    | 2.17                     | 0.43              |
| 53:1:483:A:H2'    | 53:1:484:C:H5'   | 2.00                     | 0.43              |
| 53:1:968:C:H2'    | 53:1:969:G:C8    | 2.54                     | 0.43              |
| 53:1:996:A:H2'    | 53:1:997:G:H8    | 1.83                     | 0.43              |
| 53:1:1181:U:H2'   | 53:1:1182:G:C8   | 2.54                     | 0.43              |
| 53:1:2297:A:H62   | 53:1:2319:G:H1'  | 1.84                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 53:1:2364:C:H2'   | 53:1:2365:G:O4'  | 2.18                     | 0.43              |
| 53:1:2368:C:H2'   | 53:1:2369:A:C8   | 2.53                     | 0.43              |
| 53:1:2637:U:H2'   | 53:1:2638:G:O4'  | 2.19                     | 0.43              |
| 54:2:60:C:H2'     | 54:2:61:G:C8     | 2.54                     | 0.43              |
| 2:c:57:ALA:O      | 2:c:60:VAL:HG12  | 2.18                     | 0.43              |
| 2:c:121:THR:C     | 2:c:127:PHE:HB2  | 2.44                     | 0.43              |
| 9:j:111:LYS:NZ    | 53:1:2039:U:C6   | 2.87                     | 0.43              |
| 31:G:3:VAL:HG21   | 31:G:49:PHE:HE2  | 1.83                     | 0.43              |
| 32:H:86:LEU:O     | 32:H:90:VAL:HG22 | 2.18                     | 0.43              |
| 33:I:56:GLU:O     | 33:I:59:LYS:HG2  | 2.18                     | 0.43              |
| 44:T:80:LEU:H     | 44:T:80:LEU:HD12 | 1.84                     | 0.43              |
| 50:Z:6:ARG:O      | 50:Z:7:GLU:HB2   | 2.19                     | 0.43              |
| 51:a:6:LYS:HZ2    | 53:1:2130:U:H5   | 1.59                     | 0.43              |
| 52:3:407:U:H2'    | 52:3:408:A:C8    | 2.53                     | 0.43              |
| 53:1:1013:C:H2'   | 53:1:1014:A:H8   | 1.82                     | 0.43              |
| 53:1:2296:U:C5'   | 53:1:2297:A:OP1  | 2.62                     | 0.43              |
| 55:6:17:C:H2'     | 55:6:17(A):U:C5  | 2.54                     | 0.43              |
| 2:c:19:GLY:HA2    | 15:p:78:PRO:HD2  | 2.01                     | 0.43              |
| 3:d:176:ASP:N     | 3:d:176:ASP:OD1  | 2.51                     | 0.43              |
| 9:j:41:LYS:HG3    | 9:j:43:GLU:OE1   | 2.19                     | 0.43              |
| 11:l:47:ARG:NH1   | 53:1:195:A:H5''  | 2.14                     | 0.43              |
| 19:t:77:ARG:HG3   | 53:1:63:A:O2'    | 2.19                     | 0.43              |
| 27:C:26:LYS:HD2   | 27:C:26:LYS:C    | 2.44                     | 0.43              |
| 31:G:186:VAL:HG21 | 31:G:192:PRO:HB3 | 2.01                     | 0.43              |
| 34:J:11:GLN:HB3   | 34:J:39:GLY:O    | 2.19                     | 0.43              |
| 38:N:66:VAL:HG11  | 38:N:74:GLN:HB3  | 2.01                     | 0.43              |
| 39:O:39:PRO:HA    | 39:O:73:LEU:O    | 2.19                     | 0.43              |
| 39:O:67:ILE:HG13  | 39:O:67:ILE:O    | 2.19                     | 0.43              |
| 46:V:59:GLU:OE1   | 46:V:59:GLU:N    | 2.51                     | 0.43              |
| 48:X:17:LYS:NZ    | 48:X:31:ARG:HD3  | 2.33                     | 0.43              |
| 52:3:1394:A:H3'   | 52:3:1395:C:H5'  | 2.00                     | 0.43              |
| 53:1:542:C:H2'    | 53:1:543:G:C5'   | 2.49                     | 0.43              |
| 53:1:720:U:H2'    | 53:1:721:A:H8    | 1.83                     | 0.43              |
| 53:1:784:G:OP1    | 53:1:2588:G:H5'' | 2.18                     | 0.43              |
| 53:1:941:A:O2'    | 53:1:1190:G:H4'  | 2.19                     | 0.43              |
| 53:1:1370:C:H2'   | 53:1:1371:G:O4'  | 2.18                     | 0.43              |
| 55:6:34:C:H42     | 56:4:13:A:N6     | 2.16                     | 0.43              |
| 4:e:36:ASN:O      | 4:e:151:LEU:HB2  | 2.18                     | 0.43              |
| 4:e:144:LYS:N     | 4:e:144:LYS:HD2  | 2.34                     | 0.43              |
| 6:g:37:VAL:HA     | 6:g:38:PRO:HD3   | 1.91                     | 0.43              |
| 7:h:11:ILE:O      | 7:h:15:VAL:HG23  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:h:27:VAL:CG1    | 7:h:83:ALA:HB3    | 2.48                     | 0.43              |
| 8:i:29:GLN:HE21   | 8:i:30:GLN:NE2    | 2.15                     | 0.43              |
| 11:l:109:LYS:HG2  | 11:l:126:ARG:HB3  | 2.01                     | 0.43              |
| 17:r:83:TYR:CZ    | 53:1:1187:G:H5''  | 2.53                     | 0.43              |
| 33:I:57:LYS:NZ    | 33:I:58:GLN:OE1   | 2.49                     | 0.43              |
| 36:L:113:LYS:HZ1  | 52:3:1297:G:H1'   | 1.83                     | 0.43              |
| 38:N:123:ARG:HH22 | 38:N:126:PHE:HB2  | 1.84                     | 0.43              |
| 39:O:59:LYS:HE3   | 39:O:62:ARG:HH21  | 1.84                     | 0.43              |
| 40:P:91:GLY:O     | 40:P:92:ARG:HG2   | 2.18                     | 0.43              |
| 40:P:121:ARG:HD3  | 52:3:778:G:N2     | 2.33                     | 0.43              |
| 43:S:20:PHE:O     | 43:S:21:ALA:CB    | 2.66                     | 0.43              |
| 43:S:52:ARG:HH12  | 48:X:36:ARG:HH22  | 1.66                     | 0.43              |
| 43:S:76:PHE:CZ    | 43:S:92:ILE:HD13  | 2.54                     | 0.43              |
| 53:1:158:U:H2'    | 53:1:159:G:O4'    | 2.19                     | 0.43              |
| 53:1:937:C:H2'    | 53:1:938:G:H8     | 1.83                     | 0.43              |
| 53:1:1301:A:H2'   | 53:1:1301:A:N3    | 2.33                     | 0.43              |
| 2:c:24:VAL:HG22   | 2:c:25:THR:N      | 2.34                     | 0.43              |
| 6:g:94:ILE:HD11   | 6:g:122:LEU:CD2   | 2.48                     | 0.43              |
| 8:i:79:LEU:HA     | 8:i:82:ALA:HB3    | 2.00                     | 0.43              |
| 12:m:125:PRO:HB3  | 53:1:2485:G:O3'   | 2.18                     | 0.43              |
| 13:n:54:LEU:HD11  | 13:n:65:LEU:HB3   | 2.01                     | 0.43              |
| 14:o:110:ALA:HB1  | 14:o:115:LEU:HD22 | 2.00                     | 0.43              |
| 19:t:39:THR:HG23  | 19:t:42:GLU:H     | 1.84                     | 0.43              |
| 27:C:21:THR:O     | 29:E:33:THR:OG1   | 2.35                     | 0.43              |
| 31:G:26:MET:SD    | 31:G:29:PHE:HB2   | 2.59                     | 0.43              |
| 32:H:175:HIS:ND1  | 52:3:1108:G:H5'   | 2.34                     | 0.43              |
| 34:J:44:ARG:NH2   | 34:J:70:MET:HG2   | 2.34                     | 0.43              |
| 34:J:110:MET:O    | 34:J:113:VAL:HG22 | 2.19                     | 0.43              |
| 38:N:6:TYR:HA     | 38:N:18:VAL:O     | 2.19                     | 0.43              |
| 42:R:21:ILE:N     | 42:R:21:ILE:HD12  | 2.33                     | 0.43              |
| 45:U:51:ARG:NH1   | 52:3:627:G:H5'    | 2.34                     | 0.43              |
| 47:W:32:ILE:O     | 47:W:32:ILE:HG13  | 2.17                     | 0.43              |
| 53:1:464:U:H2'    | 53:1:465:G:O4'    | 2.18                     | 0.43              |
| 53:1:780:G:H2'    | 53:1:782:A:N7     | 2.34                     | 0.43              |
| 53:1:873:C:H2'    | 53:1:874:G:H8     | 1.84                     | 0.43              |
| 53:1:940:G:H2'    | 53:1:941:A:H5''   | 2.00                     | 0.43              |
| 53:1:1991:U:H2'   | 53:1:1992:G:C5'   | 2.49                     | 0.43              |
| 53:1:2247:A:H2'   | 53:1:2248:C:C6    | 2.54                     | 0.43              |
| 2:c:6:GLY:HA3     | 2:c:29:VAL:HG22   | 2.00                     | 0.42              |
| 2:c:159:LYS:HD3   | 2:c:160:LYS:N     | 2.34                     | 0.42              |
| 3:d:14:VAL:HG22   | 3:d:15:SER:N      | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:h:42:ARG:HH22   | 53:1:1082:U:H4'   | 1.85                     | 0.42              |
| 12:m:16:ARG:HG3   | 53:1:953:G:OP2    | 2.18                     | 0.42              |
| 13:n:95:THR:OG1   | 13:n:96:ARG:N     | 2.52                     | 0.42              |
| 18:s:88:ARG:HB2   | 18:s:92:ARG:O     | 2.19                     | 0.42              |
| 23:x:43:LYS:O     | 23:x:43:LYS:HG3   | 2.19                     | 0.42              |
| 38:N:26:LYS:C     | 38:N:27:ILE:HD12  | 2.44                     | 0.42              |
| 43:S:32:ASP:O     | 43:S:40:ARG:NH1   | 2.51                     | 0.42              |
| 49:Y:7:LYS:HE3    | 49:Y:7:LYS:HB2    | 1.92                     | 0.42              |
| 52:3:971:G:H1'    | 52:3:1365:G:O2'   | 2.19                     | 0.42              |
| 52:3:1114:C:H2'   | 52:3:1115:U:O4'   | 2.18                     | 0.42              |
| 52:3:1415:G:H2'   | 52:3:1416:G:C8    | 2.54                     | 0.42              |
| 53:1:598:U:H2'    | 53:1:599:A:C8     | 2.54                     | 0.42              |
| 53:1:974:G:H1'    | 53:1:975:A:C8     | 2.54                     | 0.42              |
| 53:1:1442:U:H2'   | 53:1:1443:U:C6    | 2.54                     | 0.42              |
| 53:1:1510:G:H2'   | 53:1:1511:G:O4'   | 2.18                     | 0.42              |
| 53:1:1919:A:H2'   | 53:1:1920:C:H5'   | 2.01                     | 0.42              |
| 53:1:1956:U:H1'   | 53:1:2552:U:OP1   | 2.19                     | 0.42              |
| 53:1:2704:C:H2'   | 53:1:2705:A:O4'   | 2.19                     | 0.42              |
| 53:1:2898:U:H2'   | 53:1:2899:A:C8    | 2.54                     | 0.42              |
| 1:b:116:GLN:HE21  | 1:b:121:ALA:HA    | 1.83                     | 0.42              |
| 1:b:131:MET:HA    | 1:b:134:ILE:HD12  | 2.02                     | 0.42              |
| 3:d:164:LEU:O     | 3:d:167:VAL:HG22  | 2.19                     | 0.42              |
| 11:l:77:ILE:HD12  | 11:l:77:ILE:N     | 2.34                     | 0.42              |
| 12:m:3:GLN:HA     | 12:m:4:PRO:HD3    | 1.89                     | 0.42              |
| 12:m:59:ARG:HD2   | 12:m:59:ARG:N     | 2.27                     | 0.42              |
| 12:m:82:MET:HE1   | 53:1:956:G:H4'    | 2.01                     | 0.42              |
| 12:m:125:PRO:HB3  | 53:1:2485:G:H4'   | 2.00                     | 0.42              |
| 16:q:46:TYR:O     | 16:q:49:ARG:HG2   | 2.18                     | 0.42              |
| 31:G:58:LYS:HB2   | 31:G:58:LYS:HE3   | 1.79                     | 0.42              |
| 32:H:159:ALA:HB3  | 32:H:163:ARG:HH12 | 1.84                     | 0.42              |
| 34:J:152:VAL:HG22 | 34:J:156:ARG:HB3  | 2.00                     | 0.42              |
| 35:K:86:ARG:NH1   | 52:3:673:A:H4'    | 2.34                     | 0.42              |
| 36:L:3:ARG:HD2    | 52:3:932:C:OP1    | 2.19                     | 0.42              |
| 52:3:252:U:O2     | 52:3:252:U:H2'    | 2.19                     | 0.42              |
| 52:3:729:A:H2'    | 52:3:730:G:C8     | 2.54                     | 0.42              |
| 53:1:174:U:H2'    | 53:1:175:G:C8     | 2.54                     | 0.42              |
| 53:1:241:A:H61    | 53:1:255:A:H3'    | 1.83                     | 0.42              |
| 53:1:1026:G:H2'   | 53:1:1027:A:C8    | 2.51                     | 0.42              |
| 53:1:1893:C:H2'   | 53:1:1894:C:H5'   | 2.00                     | 0.42              |
| 53:1:2248:C:H2'   | 53:1:2249:U:H5'   | 1.99                     | 0.42              |
| 53:1:2376:A:H2'   | 53:1:2377:A:O4'   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:b:3:VAL:HG22   | 1:b:4:LYS:N       | 2.34                     | 0.42              |
| 1:b:220:ARG:HD3  | 53:1:1827:U:C5    | 2.53                     | 0.42              |
| 6:g:31:VAL:N     | 6:g:32:PRO:HD2    | 2.34                     | 0.42              |
| 7:h:58:THR:HG23  | 53:1:1107:G:H5''  | 1.97                     | 0.42              |
| 10:k:2:ILE:N     | 10:k:2:ILE:HD12   | 2.35                     | 0.42              |
| 16:q:31:TYR:HB3  | 53:1:581:C:OP1    | 2.19                     | 0.42              |
| 16:q:52:ARG:HD3  | 53:1:535:G:O2'    | 2.19                     | 0.42              |
| 17:r:27:ILE:HD12 | 17:r:27:ILE:N     | 2.34                     | 0.42              |
| 19:t:51:PHE:O    | 19:t:53:VAL:HG23  | 2.18                     | 0.42              |
| 24:y:31:GLN:HG3  | 24:y:36:GLN:HB2   | 2.01                     | 0.42              |
| 24:y:41:HIS:CG   | 53:1:96:C:H4'     | 2.55                     | 0.42              |
| 34:J:92:ARG:O    | 34:J:93:VAL:O     | 2.36                     | 0.42              |
| 34:J:105:ILE:O   | 34:J:105:ILE:HG23 | 2.19                     | 0.42              |
| 35:K:18:VAL:O    | 35:K:22:ILE:HG13  | 2.19                     | 0.42              |
| 37:M:10:LEU:HB3  | 37:M:74:ILE:HG21  | 1.99                     | 0.42              |
| 45:U:14:ARG:HA   | 45:U:42:ILE:HD13  | 2.00                     | 0.42              |
| 52:3:303:A:H2'   | 52:3:304:U:O4'    | 2.19                     | 0.42              |
| 52:3:497:G:H2'   | 52:3:498:A:C8     | 2.53                     | 0.42              |
| 52:3:505:G:H4'   | 52:3:534:U:C4     | 2.54                     | 0.42              |
| 52:3:909:A:H2'   | 52:3:910:C:O4'    | 2.18                     | 0.42              |
| 52:3:1138:G:H3'  | 52:3:1138:G:N3    | 2.34                     | 0.42              |
| 52:3:1301:U:O2   | 52:3:1301:U:C2'   | 2.66                     | 0.42              |
| 52:3:1415:G:H2'  | 52:3:1416:G:H8    | 1.84                     | 0.42              |
| 53:1:331:C:H41   | 53:1:1210:G:N2    | 2.18                     | 0.42              |
| 53:1:433:C:O2'   | 53:1:434:U:H5'    | 2.19                     | 0.42              |
| 1:b:106:PRO:HD2  | 1:b:109:LEU:HD22  | 2.00                     | 0.42              |
| 2:c:43:ASP:HB3   | 2:c:45:TYR:CE1    | 2.54                     | 0.42              |
| 3:d:154:ASP:OD1  | 3:d:157:LEU:HB3   | 2.19                     | 0.42              |
| 5:f:76:ILE:O     | 5:f:81:GLY:N      | 2.50                     | 0.42              |
| 6:g:32:PRO:HA    | 23:x:38:TRP:CG    | 2.54                     | 0.42              |
| 7:h:100:ALA:HA   | 7:h:103:ASN:ND2   | 2.35                     | 0.42              |
| 17:r:88:GLY:HA3  | 53:1:1225:G:OP1   | 2.19                     | 0.42              |
| 18:s:8:ARG:HG2   | 18:s:102:HIS:CD2  | 2.54                     | 0.42              |
| 28:D:30:VAL:HA   | 28:D:33:ARG:HH22  | 1.85                     | 0.42              |
| 34:J:80:LEU:HB2  | 34:J:122:VAL:HG12 | 2.01                     | 0.42              |
| 37:M:9:MET:HG3   | 37:M:26:MET:SD    | 2.60                     | 0.42              |
| 37:M:93:LYS:HD2  | 37:M:93:LYS:C     | 2.44                     | 0.42              |
| 43:S:8:ARG:NH2   | 52:3:1217:C:OP2   | 2.46                     | 0.42              |
| 48:X:77:ARG:NH1  | 52:3:1222:G:H5''  | 2.34                     | 0.42              |
| 52:3:410:G:H2'   | 52:3:429:U:C4     | 2.54                     | 0.42              |
| 52:3:739:C:H2'   | 52:3:740:U:O4'    | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 52:3:880:C:H2'   | 52:3:881:G:C8    | 2.54                     | 0.42              |
| 52:3:1510:C:H2'  | 52:3:1511:G:C8   | 2.54                     | 0.42              |
| 53:1:826:U:H5''  | 53:1:2429:G:P    | 2.59                     | 0.42              |
| 53:1:1045:C:H5'  | 53:1:1046:A:C5'  | 2.46                     | 0.42              |
| 53:1:1298:C:H2'  | 53:1:1299:G:O4'  | 2.19                     | 0.42              |
| 53:1:1542:U:H2'  | 53:1:1543:G:O4'  | 2.19                     | 0.42              |
| 53:1:2855:C:H2'  | 53:1:2856:A:C8   | 2.55                     | 0.42              |
| 1:b:48:ILE:HG22  | 53:1:779:U:OP1   | 2.20                     | 0.42              |
| 3:d:48:THR:H     | 3:d:51:GLU:CD    | 2.28                     | 0.42              |
| 16:q:15:LYS:O    | 16:q:19:GLN:HG3  | 2.19                     | 0.42              |
| 16:q:20:ALA:HB2  | 16:q:38:VAL:CG2  | 2.48                     | 0.42              |
| 16:q:82:LEU:HB3  | 16:q:87:VAL:HB   | 2.01                     | 0.42              |
| 18:s:25:ARG:NH2  | 53:1:520:G:H5''  | 2.34                     | 0.42              |
| 20:u:17:ASP:CG   | 20:u:20:LYS:HD2  | 2.45                     | 0.42              |
| 20:u:48:VAL:HA   | 20:u:49:PRO:HD3  | 1.88                     | 0.42              |
| 25:z:26:LEU:HD21 | 25:z:43:ILE:HG23 | 2.02                     | 0.42              |
| 33:I:97:LEU:HB2  | 33:I:134:TYR:HB3 | 2.00                     | 0.42              |
| 33:I:103:ARG:HG3 | 33:I:169:TRP:HZ2 | 1.85                     | 0.42              |
| 37:M:40:LYS:NZ   | 37:M:46:GLU:HA   | 2.35                     | 0.42              |
| 39:O:66:GLU:HG2  | 43:S:98:ALA:CB   | 2.48                     | 0.42              |
| 40:P:126:ARG:HD2 | 40:P:126:ARG:HA  | 1.90                     | 0.42              |
| 44:T:57:ARG:HG2  | 44:T:57:ARG:NH1  | 2.35                     | 0.42              |
| 48:X:35:ARG:HH11 | 52:3:1221:G:H5'' | 1.85                     | 0.42              |
| 52:3:692:U:H2'   | 52:3:694:A:OP2   | 2.20                     | 0.42              |
| 52:3:1255:G:O2'  | 52:3:1258:G:H1'  | 2.19                     | 0.42              |
| 53:1:122:G:H2'   | 53:1:123:G:O4'   | 2.20                     | 0.42              |
| 53:1:885:C:H2'   | 53:1:886:A:C8    | 2.55                     | 0.42              |
| 53:1:1558:C:H4'  | 53:1:1560:G:OP2  | 2.18                     | 0.42              |
| 53:1:2162:G:H2'  | 53:1:2163:A:C8   | 2.54                     | 0.42              |
| 53:1:2244:U:H2'  | 53:1:2245:U:O4'  | 2.20                     | 0.42              |
| 53:1:2264:C:H2'  | 53:1:2265:U:O4'  | 2.18                     | 0.42              |
| 53:1:2398:U:H2'  | 53:1:2399:G:C8   | 2.55                     | 0.42              |
| 53:1:2463:C:H2'  | 53:1:2464:G:C8   | 2.54                     | 0.42              |
| 54:2:88:C:C5'    | 54:2:89:U:OP1    | 2.67                     | 0.42              |
| 54:2:101:A:H2'   | 54:2:102:G:O4'   | 2.19                     | 0.42              |
| 4:e:98:PHE:O     | 4:e:102:LEU:HD23 | 2.20                     | 0.42              |
| 8:i:102:ARG:NH1  | 8:i:106:GLN:HB2  | 2.31                     | 0.42              |
| 13:n:59:SER:O    | 13:n:63:ARG:HG2  | 2.19                     | 0.42              |
| 16:q:91:ARG:HG3  | 16:q:91:ARG:HH11 | 1.84                     | 0.42              |
| 20:u:3:LYS:NZ    | 53:1:336:C:OP1   | 2.50                     | 0.42              |
| 24:y:56:LEU:HA   | 24:y:59:GLU:HB3  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 33:I:108:ALA:HB3  | 33:I:112:GLU:OE1 | 2.19                     | 0.42              |
| 36:L:27:ASN:ND2   | 52:3:1374:A:OP1  | 2.53                     | 0.42              |
| 38:N:12:LYS:HG2   | 52:3:1371:G:OP1  | 2.20                     | 0.42              |
| 41:Q:2:THR:HG23   | 41:Q:2:THR:O     | 2.19                     | 0.42              |
| 41:Q:36:VAL:HG13  | 41:Q:52:CYS:HB2  | 2.01                     | 0.42              |
| 51:a:65:LEU:HD23  | 51:a:68:GLY:HA2  | 2.00                     | 0.42              |
| 52:3:160:A:H2'    | 52:3:161:A:O4'   | 2.19                     | 0.42              |
| 52:3:806:C:H2'    | 52:3:807:A:C8    | 2.55                     | 0.42              |
| 53:1:167:A:H2'    | 53:1:168:G:O4'   | 2.20                     | 0.42              |
| 53:1:1758:U:H5    | 53:1:2696:U:H5'  | 1.83                     | 0.42              |
| 53:1:1772:A:H2'   | 53:1:1773:A:H4'  | 2.01                     | 0.42              |
| 53:1:2117:A:H4'   | 53:1:2149:U:OP1  | 2.20                     | 0.42              |
| 53:1:2313:C:H2'   | 53:1:2314:A:C8   | 2.54                     | 0.42              |
| 1:b:202:ARG:NH1   | 1:b:213:ARG:HH21 | 2.17                     | 0.42              |
| 2:c:48:ILE:CG2    | 2:c:82:PHE:HB2   | 2.49                     | 0.42              |
| 3:d:52:VAL:HB     | 3:d:74:LYS:HG2   | 2.01                     | 0.42              |
| 6:g:93:SER:HB2    | 6:g:123:ARG:NE   | 2.34                     | 0.42              |
| 8:i:71:LYS:HD3    | 8:i:72:THR:O     | 2.20                     | 0.42              |
| 9:j:85:LYS:NZ     | 53:1:2768:U:OP1  | 2.52                     | 0.42              |
| 12:m:12:MET:SD    | 12:m:13:HIS:O    | 2.78                     | 0.42              |
| 18:s:41:LYS:O     | 18:s:44:ALA:HB3  | 2.19                     | 0.42              |
| 28:D:34:ARG:NH1   | 53:1:467:G:OP2   | 2.46                     | 0.42              |
| 29:E:56:LEU:HD12  | 29:E:56:LEU:H    | 1.85                     | 0.42              |
| 31:G:65:LYS:HE2   | 31:G:157:PRO:HA  | 2.02                     | 0.42              |
| 32:H:181:ILE:HG13 | 32:H:202:PHE:HD1 | 1.84                     | 0.42              |
| 39:O:10:LEU:HD23  | 39:O:72:ARG:O    | 2.20                     | 0.42              |
| 42:R:58:GLU:O     | 42:R:61:LYS:HG2  | 2.20                     | 0.42              |
| 47:W:11:ARG:H     | 47:W:11:ARG:HD3  | 1.83                     | 0.42              |
| 52:3:663:A:H5'    | 52:3:836:G:OP1   | 2.20                     | 0.42              |
| 52:3:1118:U:H2'   | 52:3:1119:C:C6   | 2.55                     | 0.42              |
| 53:1:1440:U:H2'   | 53:1:1441:G:C8   | 2.55                     | 0.42              |
| 53:1:1857:G:H1'   | 53:1:1885:A:N6   | 2.34                     | 0.42              |
| 55:6:41:C:H2'     | 55:6:42:G:C8     | 2.54                     | 0.42              |
| 1:b:23:LEU:CD1    | 1:b:82:TYR:HB2   | 2.43                     | 0.42              |
| 6:g:5:LEU:CD2     | 6:g:13:GLY:HA3   | 2.50                     | 0.42              |
| 6:g:40:THR:O      | 6:g:41:LYS:C     | 2.63                     | 0.42              |
| 8:i:33:ASN:HD21   | 8:i:35:MET:HB2   | 1.83                     | 0.42              |
| 11:l:41:ARG:NH1   | 53:1:806:C:OP2   | 2.53                     | 0.42              |
| 12:m:136:MET:O    | 21:v:79:ARG:NH2  | 2.49                     | 0.42              |
| 13:n:64:ARG:NH2   | 53:1:2851:A:O3'  | 2.53                     | 0.42              |
| 15:p:77:SER:HA    | 15:p:78:PRO:HD3  | 1.91                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 27:C:22:THR:OG1  | 27:C:23:THR:N     | 2.53                     | 0.42              |
| 34:J:110:MET:HG3 | 34:J:139:THR:HG21 | 2.01                     | 0.42              |
| 36:L:138:GLU:HA  | 36:L:141:HIS:HB2  | 2.01                     | 0.42              |
| 40:P:88:PRO:HG2  | 40:P:89:GLY:H     | 1.84                     | 0.42              |
| 41:Q:3:VAL:HA    | 41:Q:6:LEU:HG     | 2.00                     | 0.42              |
| 41:Q:33:CYS:SG   | 41:Q:79:ILE:HG12  | 2.59                     | 0.42              |
| 42:R:108:ARG:CZ  | 52:3:1308:U:H5'   | 2.49                     | 0.42              |
| 44:T:52:ARG:NE   | 53:1:715:A:H61    | 2.17                     | 0.42              |
| 47:W:56:ARG:O    | 47:W:60:ARG:HG3   | 2.19                     | 0.42              |
| 49:Y:10:ALA:O    | 49:Y:14:GLU:HG2   | 2.20                     | 0.42              |
| 52:3:180:U:H2'   | 52:3:181:A:O4'    | 2.19                     | 0.42              |
| 52:3:406:G:O2'   | 52:3:407:U:H5'    | 2.20                     | 0.42              |
| 52:3:1123:U:O2'  | 52:3:1124:G:H5'   | 2.19                     | 0.42              |
| 52:3:1368:A:O2'  | 52:3:1369:C:H5'   | 2.20                     | 0.42              |
| 53:1:184:C:H2'   | 53:1:185:G:C8     | 2.54                     | 0.42              |
| 53:1:909:A:H2'   | 53:1:912:C:C5     | 2.55                     | 0.42              |
| 53:1:1373:A:C4'  | 53:1:2212:A:H1'   | 2.49                     | 0.42              |
| 53:1:1424:G:H2'  | 53:1:1425:G:O4'   | 2.20                     | 0.42              |
| 53:1:1844:C:H2'  | 53:1:1845:G:H8    | 1.83                     | 0.42              |
| 53:1:1909:C:H2'  | 53:1:1910:G:H8    | 1.85                     | 0.42              |
| 53:1:2036:C:H2'  | 53:1:2037:A:C8    | 2.55                     | 0.42              |
| 53:1:2326:C:O2'  | 53:1:2327:A:P     | 2.78                     | 0.42              |
| 55:6:16:C:O2'    | 55:6:17:C:H5'     | 2.19                     | 0.42              |
| 2:c:56:LYS:HZ1   | 53:1:2830:C:H5''  | 1.84                     | 0.42              |
| 3:d:164:LEU:HB2  | 3:d:167:VAL:HG21  | 2.01                     | 0.42              |
| 5:f:88:LEU:CD2   | 5:f:95:ALA:HB2    | 2.50                     | 0.42              |
| 6:g:8:LYS:O      | 6:g:9:VAL:C       | 2.63                     | 0.42              |
| 6:g:97:ARG:HH22  | 53:1:2220:U:H5''  | 1.75                     | 0.42              |
| 16:q:14:LYS:NZ   | 53:1:1218:G:OP2   | 2.53                     | 0.42              |
| 22:w:15:LYS:NZ   | 53:1:2261:C:H5''  | 2.35                     | 0.42              |
| 31:G:22:TRP:CZ2  | 52:3:829:G:H4'    | 2.55                     | 0.42              |
| 45:U:6:LEU:HD23  | 45:U:19:VAL:HG13  | 2.01                     | 0.42              |
| 47:W:37:LYS:HE2  | 52:3:718:A:H2     | 1.85                     | 0.42              |
| 52:3:61:G:H2'    | 52:3:62:U:O4'     | 2.19                     | 0.42              |
| 52:3:501:C:H2'   | 52:3:502:A:H8     | 1.82                     | 0.42              |
| 52:3:788:U:H2'   | 52:3:789:U:O4'    | 2.20                     | 0.42              |
| 52:3:1354:U:H2'  | 52:3:1355:G:H8    | 1.84                     | 0.42              |
| 1:b:75:ALA:O     | 1:b:114:GLN:HG3   | 2.19                     | 0.42              |
| 3:d:176:ASP:HA   | 3:d:177:PRO:HD3   | 1.87                     | 0.42              |
| 4:e:28:PRO:HB2   | 4:e:168:LEU:CD2   | 2.49                     | 0.42              |
| 10:k:64:ARG:HD3  | 10:k:102:PRO:HG2  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:r:54:VAL:HG12  | 17:r:55:ASP:CG    | 2.45                     | 0.42              |
| 20:u:42:LYS:HB2   | 53:1:499:U:H4'    | 2.01                     | 0.42              |
| 21:v:17:SER:OG    | 21:v:21:ARG:NH2   | 2.53                     | 0.42              |
| 34:J:96:GLN:HG3   | 34:J:97:PRO:HD2   | 2.02                     | 0.42              |
| 37:M:45:ILE:HD13  | 37:M:48:PHE:HB3   | 2.02                     | 0.42              |
| 38:N:17:ARG:NH1   | 52:3:1129:C:H4'   | 2.34                     | 0.42              |
| 39:O:56:HIS:ND1   | 39:O:57:VAL:HG13  | 2.34                     | 0.42              |
| 40:P:125:LYS:O    | 50:Z:34:ARG:NE    | 2.53                     | 0.42              |
| 42:R:8:ILE:HG22   | 42:R:8:ILE:O      | 2.19                     | 0.42              |
| 46:V:54:ILE:HD12  | 46:V:54:ILE:N     | 2.35                     | 0.42              |
| 52:3:982:U:H4'    | 52:3:983:A:O5'    | 2.20                     | 0.42              |
| 53:1:814:C:H5'    | 53:1:1225:G:H1'   | 2.02                     | 0.42              |
| 3:d:85:PHE:HE2    | 53:1:586:A:H4'    | 1.85                     | 0.41              |
| 6:g:89:LYS:HA     | 6:g:89:LYS:HD2    | 1.84                     | 0.41              |
| 7:h:58:THR:CG2    | 53:1:1107:G:H5'   | 2.44                     | 0.41              |
| 15:p:54:LEU:HA    | 15:p:76:HIS:HD2   | 1.84                     | 0.41              |
| 20:u:65:GLN:HB2   | 20:u:68:ASN:ND2   | 2.35                     | 0.41              |
| 23:x:48:LEU:HD21  | 23:x:77:TYR:HB2   | 2.02                     | 0.41              |
| 32:H:125:ARG:HD2  | 32:H:125:ARG:N    | 2.35                     | 0.41              |
| 34:J:17:VAL:HA    | 34:J:33:THR:O     | 2.20                     | 0.41              |
| 46:V:14:ASP:HA    | 46:V:20:ILE:HG13  | 2.02                     | 0.41              |
| 50:Z:57:LYS:HD2   | 50:Z:65:ARG:HH22  | 1.85                     | 0.41              |
| 52:3:82:G:H2'     | 52:3:83:C:H5'     | 2.02                     | 0.41              |
| 52:3:1060:U:H2'   | 52:3:1061:G:C8    | 2.53                     | 0.41              |
| 53:1:699:A:H2'    | 53:1:700:G:O4'    | 2.20                     | 0.41              |
| 53:1:1429:G:H2'   | 53:1:1430:G:C8    | 2.55                     | 0.41              |
| 1:b:60:ALA:HB3    | 1:b:62:ARG:NH1    | 2.35                     | 0.41              |
| 2:c:46:ARG:NH2    | 2:c:88:GLU:O      | 2.53                     | 0.41              |
| 4:e:70:ARG:NH2    | 53:1:2298:A:OP1   | 2.53                     | 0.41              |
| 6:g:97:ARG:NH2    | 53:1:2220:U:C5'   | 2.72                     | 0.41              |
| 8:i:12:VAL:HG12   | 8:i:13:ALA:N      | 2.34                     | 0.41              |
| 10:k:30:ARG:HD2   | 53:1:2674:G:H4'   | 2.02                     | 0.41              |
| 17:r:79:ARG:HH22  | 53:1:572:A:H5'    | 1.85                     | 0.41              |
| 18:s:14:ALA:O     | 18:s:18:ARG:HG3   | 2.20                     | 0.41              |
| 19:t:16:VAL:HG13  | 19:t:16:VAL:O     | 2.20                     | 0.41              |
| 29:E:17:GLY:HA3   | 53:1:651:G:H4'    | 2.02                     | 0.41              |
| 29:E:51:LYS:HA    | 29:E:54:LEU:HD12  | 2.01                     | 0.41              |
| 32:H:113:LYS:HA   | 32:H:184:ASN:OD1  | 2.18                     | 0.41              |
| 32:H:152:VAL:HG23 | 32:H:197:VAL:HG22 | 2.02                     | 0.41              |
| 36:L:76:SER:HB2   | 36:L:85:GLN:NE2   | 2.35                     | 0.41              |
| 37:M:82:LEU:HD11  | 46:V:33:TYR:O     | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 38:N:105:ARG:C   | 38:N:105:ARG:HD3 | 2.45                     | 0.41              |
| 40:P:71:ASP:O    | 40:P:72:ALA:HB3  | 2.20                     | 0.41              |
| 44:T:46:LYS:O    | 44:T:47:LYS:HG3  | 2.20                     | 0.41              |
| 44:T:50:HIS:CE1  | 52:3:667:G:H4'   | 2.55                     | 0.41              |
| 44:T:63:ARG:HA   | 44:T:66:LEU:HD12 | 2.01                     | 0.41              |
| 47:W:66:LEU:HD23 | 47:W:66:LEU:HA   | 1.89                     | 0.41              |
| 48:X:30:LEU:HB2  | 48:X:48:ILE:HG22 | 2.02                     | 0.41              |
| 52:3:1139:G:H5'' | 52:3:1140:C:H5   | 1.85                     | 0.41              |
| 52:3:1397:C:N4   | 56:4:22:A:H2'    | 2.35                     | 0.41              |
| 53:1:828:U:H2'   | 53:1:829:A:C8    | 2.55                     | 0.41              |
| 53:1:2114:A:H2'  | 53:1:2114:A:N3   | 2.35                     | 0.41              |
| 53:1:2354:C:H2'  | 53:1:2355:G:H8   | 1.85                     | 0.41              |
| 53:1:2593:U:H2'  | 53:1:2594:C:C6   | 2.55                     | 0.41              |
| 7:h:54:VAL:HG22  | 7:h:54:VAL:O     | 2.20                     | 0.41              |
| 13:n:36:THR:OG1  | 13:n:37:THR:N    | 2.49                     | 0.41              |
| 14:o:27:VAL:HG22 | 14:o:28:VAL:N    | 2.35                     | 0.41              |
| 17:r:40:MET:SD   | 17:r:48:LYS:HA   | 2.60                     | 0.41              |
| 19:t:44:LYS:HG2  | 19:t:55:VAL:HG11 | 2.01                     | 0.41              |
| 20:u:32:LYS:NZ   | 53:1:478:A:O3'   | 2.52                     | 0.41              |
| 21:v:83:LYS:HA   | 21:v:84:PRO:HD3  | 1.92                     | 0.41              |
| 32:H:78:LYS:C    | 32:H:79:LYS:HG3  | 2.45                     | 0.41              |
| 37:M:113:ARG:HA  | 37:M:116:ARG:NE  | 2.31                     | 0.41              |
| 39:O:42:LEU:HA   | 39:O:43:PRO:HD2  | 1.75                     | 0.41              |
| 41:Q:40:THR:HA   | 41:Q:41:PRO:HD3  | 1.93                     | 0.41              |
| 42:R:13:HIS:O    | 42:R:16:ILE:HG22 | 2.19                     | 0.41              |
| 42:R:104:ASN:O   | 42:R:105:ALA:HB3 | 2.20                     | 0.41              |
| 42:R:108:ARG:NH2 | 52:3:1308:U:H5'' | 2.35                     | 0.41              |
| 45:U:35:ARG:HH22 | 52:3:627:G:P     | 2.43                     | 0.41              |
| 50:Z:36:PHE:HB2  | 50:Z:40:PRO:HD3  | 2.01                     | 0.41              |
| 52:3:629:A:H2'   | 52:3:630:A:O4'   | 2.20                     | 0.41              |
| 52:3:952:U:H2'   | 52:3:953:G:C8    | 2.55                     | 0.41              |
| 53:1:680:C:H2'   | 53:1:681:G:H8    | 1.86                     | 0.41              |
| 53:1:742:A:H2'   | 53:1:743:A:H8    | 1.85                     | 0.41              |
| 53:1:912:C:O2'   | 53:1:913:U:H5'   | 2.20                     | 0.41              |
| 53:1:1270:C:H5'' | 53:1:1271:G:O5'  | 2.20                     | 0.41              |
| 53:1:1430:G:H2'  | 53:1:1431:A:C8   | 2.56                     | 0.41              |
| 53:1:1912:A:N6   | 53:1:1917:U:H3   | 2.17                     | 0.41              |
| 53:1:2788:C:H2'  | 53:1:2789:C:C6   | 2.54                     | 0.41              |
| 1:b:213:ARG:CZ   | 53:1:1566:A:H5'  | 2.50                     | 0.41              |
| 4:e:91:ARG:HA    | 4:e:95:MET:HB3   | 2.01                     | 0.41              |
| 5:f:10:VAL:O     | 5:f:10:VAL:HG13  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:h:67:THR:HG21   | 7:h:75:ALA:HB2   | 2.01                     | 0.41              |
| 17:r:84:ARG:NH2   | 17:r:86:GLN:HG2  | 2.34                     | 0.41              |
| 31:G:170:ILE:HD11 | 52:3:1101:A:OP1  | 2.21                     | 0.41              |
| 34:J:34:ALA:HB2   | 34:J:58:ALA:HB1  | 2.02                     | 0.41              |
| 34:J:95:MET:HA    | 34:J:124:ALA:HA  | 2.01                     | 0.41              |
| 37:M:44:PHE:O     | 37:M:63:LYS:HB2  | 2.19                     | 0.41              |
| 37:M:63:LYS:HB3   | 37:M:63:LYS:HE2  | 1.83                     | 0.41              |
| 38:N:22:PRO:HA    | 38:N:60:LEU:HA   | 2.02                     | 0.41              |
| 47:W:53:GLN:HA    | 47:W:56:ARG:HB2  | 2.03                     | 0.41              |
| 48:X:38:THR:HG22  | 48:X:69:LYS:HG2  | 2.03                     | 0.41              |
| 49:Y:26:MET:HE2   | 52:3:1457:G:O2'  | 2.20                     | 0.41              |
| 50:Z:53:LYS:HD2   | 50:Z:53:LYS:HA   | 1.89                     | 0.41              |
| 52:3:514:C:H2'    | 52:3:515:G:C8    | 2.55                     | 0.41              |
| 52:3:701:U:H4'    | 52:3:703:G:H1'   | 2.02                     | 0.41              |
| 52:3:763:G:H2'    | 52:3:764:C:C6    | 2.55                     | 0.41              |
| 52:3:1137:C:H5'   | 52:3:1138:G:H5'  | 2.03                     | 0.41              |
| 53:1:1077:A:H2'   | 53:1:1078:U:H5'  | 2.01                     | 0.41              |
| 53:1:1297:C:OP1   | 53:1:2710:C:H4'  | 2.20                     | 0.41              |
| 53:1:2023:C:H4'   | 53:1:2617:U:O3'  | 2.21                     | 0.41              |
| 53:1:2789:C:H2'   | 53:1:2790:U:H5'  | 2.02                     | 0.41              |
| 54:2:95:U:H2'     | 54:2:96:G:C8     | 2.56                     | 0.41              |
| 55:6:62:C:H2'     | 55:6:63:G:C8     | 2.55                     | 0.41              |
| 1:b:208:GLY:C     | 1:b:210:ALA:N    | 2.78                     | 0.41              |
| 4:e:126:ASN:HD21  | 4:e:154:THR:HG22 | 1.85                     | 0.41              |
| 6:g:21:VAL:HG22   | 6:g:22:LYS:H     | 1.83                     | 0.41              |
| 12:m:64:TRP:N     | 12:m:104:GLU:O   | 2.52                     | 0.41              |
| 18:s:68:ASP:OD1   | 18:s:68:ASP:N    | 2.54                     | 0.41              |
| 41:Q:1:ALA:O      | 41:Q:2:THR:C     | 2.62                     | 0.41              |
| 47:W:33:THR:OG1   | 47:W:34:GLU:N    | 2.53                     | 0.41              |
| 51:a:166:ASP:HB3  | 53:1:2122:U:H4'  | 2.03                     | 0.41              |
| 51:a:214:ILE:HD12 | 51:a:214:ILE:N   | 2.35                     | 0.41              |
| 52:3:505:G:OP2    | 52:3:535:A:H5'   | 2.21                     | 0.41              |
| 52:3:742:G:H2'    | 52:3:743:A:H8    | 1.86                     | 0.41              |
| 52:3:950:U:H2'    | 52:3:951:G:C8    | 2.55                     | 0.41              |
| 52:3:952:U:H2'    | 52:3:953:G:H8    | 1.85                     | 0.41              |
| 53:1:445:C:O2'    | 53:1:446:G:H5'   | 2.21                     | 0.41              |
| 53:1:467:G:H4'    | 53:1:796:C:O2'   | 2.20                     | 0.41              |
| 53:1:560:C:H2'    | 53:1:561:G:O4'   | 2.20                     | 0.41              |
| 53:1:2146:C:H4'   | 53:1:2147:A:C5   | 2.55                     | 0.41              |
| 53:1:2185:U:H2'   | 53:1:2186:G:C8   | 2.55                     | 0.41              |
| 53:1:2613:U:O2'   | 53:1:2614:A:H5'  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:2636:C:H2'   | 53:1:2637:U:H6    | 1.86                     | 0.41              |
| 56:4:17:U:H2'     | 56:4:18:G:C8      | 2.56                     | 0.41              |
| 1:b:140:VAL:HG12  | 1:b:141:HIS:H     | 1.85                     | 0.41              |
| 3:d:155:GLU:HG2   | 3:d:156:ASN:N     | 2.35                     | 0.41              |
| 6:g:65:ALA:O      | 6:g:68:ARG:HB3    | 2.21                     | 0.41              |
| 8:i:89:SER:HA     | 8:i:135:MET:O     | 2.20                     | 0.41              |
| 10:k:35:VAL:HG21  | 10:k:106:GLU:HB3  | 2.01                     | 0.41              |
| 10:k:104:THR:HG22 | 10:k:105:ARG:N    | 2.36                     | 0.41              |
| 12:m:132:THR:HG22 | 12:m:133:LYS:H    | 1.85                     | 0.41              |
| 13:n:69:ARG:C     | 13:n:71:ARG:H     | 2.28                     | 0.41              |
| 17:r:47:VAL:O     | 17:r:47:VAL:HG13  | 2.21                     | 0.41              |
| 17:r:78:ARG:HH22  | 53:1:990:A:H61    | 1.68                     | 0.41              |
| 20:u:54:PRO:HG2   | 20:u:55:GLY:H     | 1.85                     | 0.41              |
| 22:w:34:VAL:HG11  | 22:w:41:PHE:CD2   | 2.55                     | 0.41              |
| 30:F:10:LEU:HB2   | 30:F:14:CYS:SG    | 2.61                     | 0.41              |
| 33:I:108:ALA:HA   | 33:I:164:ARG:HH22 | 1.86                     | 0.41              |
| 34:J:54:GLU:HB3   | 34:J:57:ALA:CB    | 2.50                     | 0.41              |
| 41:Q:112:ALA:HB2  | 52:3:503:C:OP2    | 2.20                     | 0.41              |
| 42:R:65:GLU:O     | 42:R:68:LEU:HG    | 2.21                     | 0.41              |
| 44:T:86:LEU:O     | 44:T:87:ARG:HB3   | 2.20                     | 0.41              |
| 45:U:73:ALA:O     | 45:U:76:LYS:HB3   | 2.20                     | 0.41              |
| 49:Y:59:ARG:HG2   | 49:Y:63:LYS:HZ2   | 1.85                     | 0.41              |
| 52:3:57:G:H2'     | 52:3:58:C:O4'     | 2.21                     | 0.41              |
| 52:3:897:C:H2'    | 52:3:898:G:C8     | 2.55                     | 0.41              |
| 52:3:1199:U:H2'   | 52:3:1200:C:H5'   | 2.02                     | 0.41              |
| 53:1:869:G:H2'    | 53:1:870:U:O4'    | 2.20                     | 0.41              |
| 53:1:1551:A:H2'   | 53:1:1552:A:O4'   | 2.21                     | 0.41              |
| 53:1:1672:A:C2    | 53:1:2582:G:H5'   | 2.56                     | 0.41              |
| 53:1:2126:A:H2'   | 53:1:2162:G:C2    | 2.55                     | 0.41              |
| 53:1:2286:G:H4'   | 53:1:2287:A:O4'   | 2.20                     | 0.41              |
| 53:1:2317:A:H2'   | 53:1:2318:G:O4'   | 2.20                     | 0.41              |
| 57:7:27:G:H2'     | 57:7:28:G:C8      | 2.56                     | 0.41              |
| 1:b:38:LYS:HD2    | 1:b:38:LYS:HA     | 1.95                     | 0.41              |
| 2:c:122:VAL:HA    | 2:c:127:PHE:H     | 1.86                     | 0.41              |
| 2:c:124:ARG:HA    | 2:c:165:MET:SD    | 2.61                     | 0.41              |
| 3:d:44:ARG:NH1    | 53:1:1248:G:OP1   | 2.53                     | 0.41              |
| 10:k:99:ILE:HD12  | 10:k:99:ILE:N     | 2.35                     | 0.41              |
| 16:q:10:ARG:CZ    | 53:1:1216:G:H5''  | 2.51                     | 0.41              |
| 17:r:19:THR:HA    | 17:r:97:LYS:HA    | 2.03                     | 0.41              |
| 20:u:43:LYS:HA    | 53:1:481:G:OP2    | 2.20                     | 0.41              |
| 22:w:74:LYS:HD2   | 22:w:74:LYS:H     | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:x:71:ARG:HG2   | 23:x:71:ARG:HH11  | 1.85                     | 0.41              |
| 24:y:1:MET:HG3    | 24:y:4:LYS:HE3    | 2.01                     | 0.41              |
| 33:I:119:HIS:CD2  | 52:3:438:U:H4'    | 2.56                     | 0.41              |
| 34:J:104:ILE:O    | 34:J:104:ILE:HG23 | 2.21                     | 0.41              |
| 34:J:123:LEU:HD21 | 52:3:7:A:N7       | 2.36                     | 0.41              |
| 36:L:122:GLU:HA   | 36:L:125:ASP:HB2  | 2.01                     | 0.41              |
| 43:S:84:ARG:C     | 43:S:86:ALA:H     | 2.28                     | 0.41              |
| 52:3:70:U:H4'     | 52:3:71:A:C8      | 2.55                     | 0.41              |
| 52:3:144:G:H2'    | 52:3:145:G:O4'    | 2.21                     | 0.41              |
| 52:3:231:U:H2'    | 52:3:232:G:H8     | 1.86                     | 0.41              |
| 52:3:396:C:H2'    | 52:3:397:A:H5''   | 2.02                     | 0.41              |
| 52:3:406:G:H2'    | 52:3:407:U:C6     | 2.56                     | 0.41              |
| 52:3:939:G:H21    | 52:3:1375:A:H2    | 1.68                     | 0.41              |
| 53:1:818:G:C2'    | 53:1:819:A:H5''   | 2.51                     | 0.41              |
| 53:1:1035:U:H2'   | 53:1:1036:G:C8    | 2.56                     | 0.41              |
| 53:1:1539:U:H2'   | 53:1:1540:G:H8    | 1.84                     | 0.41              |
| 53:1:1570:A:H2'   | 53:1:1571:A:C8    | 2.55                     | 0.41              |
| 53:1:1697:G:H4'   | 53:1:1978:A:H5''  | 2.01                     | 0.41              |
| 53:1:1775:U:H2'   | 53:1:1776:G:O4'   | 2.21                     | 0.41              |
| 53:1:1827:U:H2'   | 53:1:1828:G:O4'   | 2.21                     | 0.41              |
| 53:1:2471:A:H2'   | 53:1:2472:G:O4'   | 2.21                     | 0.41              |
| 2:c:132:ALA:HA    | 2:c:140:HIS:ND1   | 2.36                     | 0.41              |
| 9:j:81:ILE:CG2    | 9:j:82:GLY:H      | 2.19                     | 0.41              |
| 11:l:52:GLY:C     | 11:l:54:GLN:H     | 2.29                     | 0.41              |
| 11:l:101:ILE:HG13 | 11:l:102:GLY:H    | 1.85                     | 0.41              |
| 14:o:15:ARG:NH2   | 54:2:8:C:OP1      | 2.54                     | 0.41              |
| 16:q:25:GLY:HA2   | 53:1:18:U:OP1     | 2.20                     | 0.41              |
| 31:G:32:GLY:HA3   | 31:G:34:ARG:HH12  | 1.85                     | 0.41              |
| 32:H:166:TRP:CD1  | 32:H:166:TRP:H    | 2.39                     | 0.41              |
| 34:J:107:GLY:HA2  | 52:3:8:A:H1'      | 2.03                     | 0.41              |
| 35:K:15:SER:O     | 35:K:18:VAL:HG23  | 2.21                     | 0.41              |
| 36:L:91:ARG:NE    | 36:L:92:PRO:HD2   | 2.36                     | 0.41              |
| 37:M:45:ILE:CD1   | 37:M:48:PHE:HB3   | 2.50                     | 0.41              |
| 42:R:32:ILE:HG23  | 42:R:58:GLU:HG3   | 2.02                     | 0.41              |
| 43:S:82:LYS:HE2   | 43:S:82:LYS:HA    | 2.03                     | 0.41              |
| 48:X:17:LYS:HZ2   | 48:X:31:ARG:HD3   | 1.86                     | 0.41              |
| 49:Y:84:LYS:HE3   | 49:Y:84:LYS:HB3   | 1.92                     | 0.41              |
| 52:3:309:A:H2'    | 52:3:310:G:H8     | 1.86                     | 0.41              |
| 52:3:1354:U:H2'   | 52:3:1355:G:C8    | 2.55                     | 0.41              |
| 53:1:1339:G:N2    | 53:1:1603:A:H1'   | 2.36                     | 0.41              |
| 53:1:2464:G:H2'   | 53:1:2465:C:O4'   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 53:1:2730:C:O2'   | 53:1:2731:G:H5'  | 2.21                     | 0.41              |
| 53:1:2861:U:H2'   | 53:1:2862:G:C8   | 2.55                     | 0.41              |
| 1:b:43:ASN:OD1    | 1:b:47:ARG:N     | 2.50                     | 0.41              |
| 1:b:155:ARG:HB2   | 53:1:1818:U:H5'  | 2.02                     | 0.41              |
| 3:d:29:HIS:HA     | 3:d:32:VAL:HG12  | 2.02                     | 0.41              |
| 7:h:33:VAL:HA     | 53:1:1055:G:H4'  | 2.03                     | 0.41              |
| 8:i:56:VAL:HG22   | 8:i:57:VAL:N     | 2.35                     | 0.41              |
| 11:l:61:LEU:O     | 29:E:12:ARG:HD3  | 2.20                     | 0.41              |
| 11:l:63:LYS:HA    | 29:E:12:ARG:HA   | 2.02                     | 0.41              |
| 12:m:12:MET:CE    | 12:m:71:LYS:HE3  | 2.50                     | 0.41              |
| 12:m:34:LYS:HA    | 12:m:101:VAL:HA  | 2.02                     | 0.41              |
| 18:s:66:ILE:HD12  | 18:s:69:LEU:CD1  | 2.50                     | 0.41              |
| 27:C:14:ALA:HB3   | 27:C:16:THR:HG22 | 2.03                     | 0.41              |
| 27:C:22:THR:HG21  | 53:1:2286:G:O6   | 2.20                     | 0.41              |
| 28:D:40:ALA:O     | 28:D:42:LEU:HD12 | 2.21                     | 0.41              |
| 33:I:9:LYS:HD2    | 52:3:428:G:C5'   | 2.49                     | 0.41              |
| 33:I:48:SER:OG    | 33:I:49:ASP:N    | 2.53                     | 0.41              |
| 33:I:195:ASN:ND2  | 33:I:197:HIS:HB3 | 2.36                     | 0.41              |
| 33:I:195:ASN:HD21 | 33:I:197:HIS:HB3 | 1.86                     | 0.41              |
| 38:N:10:ARG:HG3   | 38:N:105:ARG:NH2 | 2.35                     | 0.41              |
| 39:O:88:MET:O     | 39:O:89:ARG:HG2  | 2.21                     | 0.41              |
| 45:U:13:LYS:NZ    | 52:3:392:C:H4'   | 2.36                     | 0.41              |
| 48:X:35:ARG:NH2   | 48:X:71:GLY:O    | 2.49                     | 0.41              |
| 48:X:44:ILE:HD13  | 48:X:63:ASP:HA   | 2.02                     | 0.41              |
| 48:X:76:THR:OG1   | 48:X:77:ARG:N    | 2.53                     | 0.41              |
| 49:Y:53:MET:SD    | 49:Y:53:MET:C    | 3.04                     | 0.41              |
| 50:Z:11:PHE:O     | 50:Z:13:VAL:N    | 2.54                     | 0.41              |
| 51:a:8:MET:SD     | 51:a:8:MET:N     | 2.91                     | 0.41              |
| 52:3:513:C:H2'    | 52:3:514:C:C6    | 2.56                     | 0.41              |
| 52:3:536:C:H2'    | 52:3:537:G:C8    | 2.56                     | 0.41              |
| 52:3:730:G:C2'    | 52:3:731:G:H5'   | 2.50                     | 0.41              |
| 52:3:1204:A:H2'   | 52:3:1205:U:O4'  | 2.21                     | 0.41              |
| 52:3:1251:A:H2'   | 52:3:1252:A:O4'  | 2.20                     | 0.41              |
| 52:3:1293:C:H2'   | 52:3:1294:G:C8   | 2.56                     | 0.41              |
| 53:1:150:U:H2'    | 53:1:151:C:C6    | 2.55                     | 0.41              |
| 53:1:621:A:C2'    | 53:1:622:G:H5'   | 2.51                     | 0.41              |
| 53:1:660:C:H2'    | 53:1:661:A:H8    | 1.85                     | 0.41              |
| 53:1:1306:C:N4    | 53:1:1606:C:H2'  | 2.36                     | 0.41              |
| 53:1:2296:U:H4'   | 53:1:2297:A:O5'  | 2.20                     | 0.41              |
| 53:1:2329:U:H2'   | 53:1:2330:G:C8   | 2.56                     | 0.41              |
| 53:1:2818:U:H4'   | 53:1:2837:A:H4'  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:2853:C:H2'   | 53:1:2854:G:H8    | 1.86                     | 0.41              |
| 57:7:64:A:H2'     | 57:7:65:G:C8      | 2.56                     | 0.41              |
| 1:b:94:LEU:HD12   | 1:b:100:ARG:HG2   | 2.03                     | 0.41              |
| 1:b:159:THR:H     | 1:b:194:VAL:HB    | 1.86                     | 0.41              |
| 1:b:160:TYR:CB    | 1:b:193:GLU:HG2   | 2.44                     | 0.41              |
| 1:b:257:ARG:NH1   | 1:b:259:ASN:HD22  | 2.18                     | 0.41              |
| 2:c:40:LEU:HA     | 2:c:44:GLY:C      | 2.46                     | 0.41              |
| 3:d:164:LEU:HB2   | 3:d:167:VAL:CG2   | 2.51                     | 0.41              |
| 8:i:118:GLY:HA2   | 53:1:1082:U:H5'   | 2.03                     | 0.41              |
| 8:i:131:THR:O     | 8:i:135:MET:HG2   | 2.21                     | 0.41              |
| 9:j:114:LEU:HD22  | 53:1:557:C:O2'    | 2.21                     | 0.41              |
| 14:o:101:GLY:HA3  | 54:2:49:C:OP1     | 2.21                     | 0.41              |
| 15:p:61:ARG:HD3   | 15:p:99:LEU:HD23  | 2.03                     | 0.41              |
| 15:p:102:ARG:HD3  | 15:p:106:ALA:O    | 2.19                     | 0.41              |
| 20:u:42:LYS:HD2   | 53:1:499:U:H5''   | 2.01                     | 0.41              |
| 20:u:73:ASN:HD22  | 20:u:76:THR:H     | 1.68                     | 0.41              |
| 23:x:12:VAL:HG23  | 23:x:28:PHE:HB2   | 2.03                     | 0.41              |
| 24:y:43:LEU:HD23  | 53:1:61:C:H5''    | 2.02                     | 0.41              |
| 32:H:115:VAL:O    | 32:H:119:ILE:HG13 | 2.20                     | 0.41              |
| 32:H:196:GLY:H    | 52:3:1057:G:H4'   | 1.86                     | 0.41              |
| 34:J:114:LEU:HD13 | 34:J:122:VAL:HG21 | 2.02                     | 0.41              |
| 34:J:133:ILE:HG23 | 34:J:134:ASN:H    | 1.85                     | 0.41              |
| 36:L:108:ARG:HA   | 36:L:108:ARG:HD3  | 1.81                     | 0.41              |
| 39:O:46:LYS:HG2   | 39:O:68:ARG:HA    | 2.02                     | 0.41              |
| 41:Q:65:TYR:OH    | 52:3:522:C:OP2    | 2.39                     | 0.41              |
| 42:R:100:ARG:HG2  | 52:3:950:U:C5     | 2.56                     | 0.41              |
| 46:V:44:HIS:HB2   | 46:V:70:LYS:HA    | 2.02                     | 0.41              |
| 49:Y:54:GLN:N     | 49:Y:55:PRO:HD2   | 2.35                     | 0.41              |
| 51:a:213:SER:C    | 51:a:214:ILE:HD12 | 2.46                     | 0.41              |
| 52:3:405:U:C3'    | 52:3:406:G:H5'    | 2.44                     | 0.41              |
| 53:1:2121:G:H2'   | 53:1:2122:U:O4'   | 2.20                     | 0.41              |
| 53:1:2329:U:H2'   | 53:1:2330:G:H8    | 1.86                     | 0.41              |
| 53:1:2821:A:H2    | 53:1:2826:A:H61   | 1.67                     | 0.41              |
| 53:1:2860:A:H2'   | 53:1:2861:U:H5'   | 2.03                     | 0.41              |
| 57:7:44:G:C3'     | 57:7:45:U:H5''    | 2.50                     | 0.41              |
| 1:b:141:HIS:CE1   | 1:b:190:THR:HB    | 2.55                     | 0.40              |
| 2:c:179:ARG:HB3   | 2:c:188:LEU:HD12  | 2.03                     | 0.40              |
| 4:e:134:GLN:HB3   | 4:e:149:ARG:O     | 2.19                     | 0.40              |
| 4:e:175:PRO:O     | 4:e:176:PHE:HB2   | 2.21                     | 0.40              |
| 6:g:5:LEU:HD12    | 6:g:5:LEU:N       | 2.35                     | 0.40              |
| 7:h:118:ILE:O     | 7:h:118:ILE:CG2   | 2.68                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:i:109:ALA:HA   | 8:i:112:LYS:HB2   | 2.03                     | 0.40              |
| 9:j:85:LYS:NZ    | 53:1:2768:U:H5''  | 2.35                     | 0.40              |
| 10:k:54:LYS:HE3  | 10:k:54:LYS:HB3   | 1.90                     | 0.40              |
| 15:p:98:TYR:O    | 15:p:101:GLU:HG2  | 2.21                     | 0.40              |
| 18:s:77:ASP:OD1  | 18:s:77:ASP:N     | 2.52                     | 0.40              |
| 20:u:44:HIS:HB2  | 53:1:482:A:H5''   | 2.03                     | 0.40              |
| 21:v:68:LYS:HG3  | 21:v:70:ILE:HG13  | 2.03                     | 0.40              |
| 24:y:4:LYS:O     | 24:y:7:ARG:NH1    | 2.54                     | 0.40              |
| 31:G:89:PHE:HD1  | 31:G:150:ILE:HA   | 1.85                     | 0.40              |
| 31:G:100:LEU:HA  | 31:G:156:LEU:HD11 | 2.03                     | 0.40              |
| 32:H:196:GLY:HA3 | 52:3:1057:G:O3'   | 2.20                     | 0.40              |
| 33:I:53:GLN:HA   | 33:I:198:LEU:HD21 | 2.02                     | 0.40              |
| 37:M:49:LYS:H    | 37:M:59:GLU:HG3   | 1.86                     | 0.40              |
| 37:M:66:GLN:HB3  | 37:M:67:GLY:H     | 1.73                     | 0.40              |
| 37:M:87:ARG:HG2  | 37:M:88:LYS:H     | 1.86                     | 0.40              |
| 39:O:44:THR:HG23 | 39:O:69:THR:O     | 2.22                     | 0.40              |
| 40:P:12:ARG:HG3  | 40:P:75:GLU:OE1   | 2.21                     | 0.40              |
| 42:R:24:VAL:HG23 | 42:R:28:ARG:CG    | 2.51                     | 0.40              |
| 46:V:37:ILE:HB   | 46:V:39:ARG:NE    | 2.36                     | 0.40              |
| 48:X:7:GLY:HA2   | 48:X:8:PRO:HD3    | 1.93                     | 0.40              |
| 49:Y:35:TYR:HD1  | 49:Y:38:ILE:HD12  | 1.87                     | 0.40              |
| 52:3:24:U:H2'    | 52:3:25:C:C6      | 2.56                     | 0.40              |
| 52:3:51:A:H4'    | 52:3:52:C:H5''    | 2.02                     | 0.40              |
| 52:3:1081:A:H2'  | 52:3:1082:A:C8    | 2.56                     | 0.40              |
| 53:1:435:C:H2'   | 53:1:436:C:H5'    | 2.02                     | 0.40              |
| 53:1:1013:C:H2'  | 53:1:1014:A:C8    | 2.56                     | 0.40              |
| 53:1:1916:A:H2'  | 53:1:1917:U:C6    | 2.56                     | 0.40              |
| 53:1:2542:A:H4'  | 53:1:2543:G:H8    | 1.85                     | 0.40              |
| 53:1:2569:G:H2'  | 53:1:2570:G:H8    | 1.85                     | 0.40              |
| 53:1:2832:U:H1'  | 53:1:2834:G:C2    | 2.57                     | 0.40              |
| 2:c:156:PHE:O    | 53:1:2619:C:H4'   | 2.21                     | 0.40              |
| 11:l:23:ILE:HG23 | 17:r:82:HIS:CD2   | 2.56                     | 0.40              |
| 15:p:93:LYS:HA   | 53:1:2848:G:C5'   | 2.51                     | 0.40              |
| 18:s:25:ARG:HD3  | 18:s:25:ARG:C     | 2.46                     | 0.40              |
| 20:u:10:VAL:CG2  | 20:u:69:VAL:HB    | 2.51                     | 0.40              |
| 25:z:4:ILE:HD11  | 25:z:56:VAL:CG1   | 2.51                     | 0.40              |
| 31:G:131:LYS:CE  | 52:3:1159:U:H3'   | 2.51                     | 0.40              |
| 32:H:178:ARG:HG2 | 32:H:206:ILE:HA   | 2.02                     | 0.40              |
| 36:L:4:ARG:N     | 36:L:4:ARG:CD     | 2.83                     | 0.40              |
| 38:N:30:ASN:HD21 | 38:N:66:VAL:H     | 1.70                     | 0.40              |
| 38:N:105:ARG:NE  | 52:3:1117:A:O3'   | 2.54                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 43:S:72:PHE:CE2   | 43:S:77:GLY:HA2  | 2.56                     | 0.40              |
| 49:Y:80:ALA:HA    | 49:Y:83:ASN:ND2  | 2.34                     | 0.40              |
| 52:3:195:A:H2'    | 52:3:196:A:C8    | 2.56                     | 0.40              |
| 52:3:1217:C:H2'   | 52:3:1218:C:O4'  | 2.21                     | 0.40              |
| 53:1:917:A:H5''   | 53:1:2268:A:H61  | 1.86                     | 0.40              |
| 53:1:1319:C:O2'   | 53:1:1320:C:H5'  | 2.22                     | 0.40              |
| 53:1:1330:C:H2'   | 53:1:1331:G:H8   | 1.87                     | 0.40              |
| 53:1:1355:G:H2'   | 53:1:1356:G:H8   | 1.86                     | 0.40              |
| 53:1:2630:G:H2'   | 53:1:2631:G:C8   | 2.56                     | 0.40              |
| 1:b:136:VAL:HG13  | 1:b:164:VAL:O    | 2.21                     | 0.40              |
| 1:b:140:VAL:HG12  | 1:b:141:HIS:N    | 2.37                     | 0.40              |
| 11:l:62:PRO:HG2   | 29:E:24:LYS:HB3  | 2.02                     | 0.40              |
| 21:v:18:ARG:HH21  | 54:2:78:A:P      | 2.44                     | 0.40              |
| 28:D:14:ARG:HD3   | 53:1:771:G:OP1   | 2.21                     | 0.40              |
| 33:I:9:LYS:NZ     | 52:3:428:G:H3'   | 2.37                     | 0.40              |
| 36:L:26:VAL:HG22  | 36:L:42:VAL:HG21 | 2.03                     | 0.40              |
| 36:L:27:ASN:HA    | 36:L:30:MET:CB   | 2.51                     | 0.40              |
| 36:L:74:VAL:HB    | 36:L:85:GLN:HB3  | 2.02                     | 0.40              |
| 36:L:94:ARG:HG2   | 36:L:98:LEU:HD13 | 2.03                     | 0.40              |
| 38:N:48:ARG:HA    | 38:N:51:LEU:HB2  | 2.04                     | 0.40              |
| 39:O:59:LYS:HD2   | 52:3:973:G:OP1   | 2.22                     | 0.40              |
| 41:Q:106:VAL:HG23 | 41:Q:116:TYR:HB3 | 2.03                     | 0.40              |
| 52:3:70:U:H2'     | 52:3:94:G:C6     | 2.57                     | 0.40              |
| 52:3:314:C:O2'    | 52:3:315:A:H5'   | 2.21                     | 0.40              |
| 52:3:665:A:N3     | 52:3:732:C:H2'   | 2.36                     | 0.40              |
| 52:3:684:U:H2'    | 52:3:685:G:O4'   | 2.21                     | 0.40              |
| 52:3:759:A:H2'    | 52:3:760:G:H5'   | 2.03                     | 0.40              |
| 52:3:1033:G:C3'   | 52:3:1034:G:H5'' | 2.51                     | 0.40              |
| 53:1:43:G:H2'     | 53:1:44:A:O4'    | 2.21                     | 0.40              |
| 53:1:741:U:H2'    | 53:1:742:A:C8    | 2.55                     | 0.40              |
| 53:1:1561:C:H2'   | 53:1:1562:U:C6   | 2.56                     | 0.40              |
| 54:2:5:U:H2'      | 54:2:6:G:C8      | 2.56                     | 0.40              |
| 55:6:17:C:H2'     | 55:6:17(A):U:H5  | 1.86                     | 0.40              |
| 1:b:42:ARG:HA     | 1:b:42:ARG:HD3   | 1.96                     | 0.40              |
| 1:b:85:ASN:HD22   | 1:b:85:ASN:HA    | 1.67                     | 0.40              |
| 1:b:200:MET:HB2   | 53:1:1820:U:C2   | 2.57                     | 0.40              |
| 4:e:23:SER:HB3    | 4:e:26:GLN:HE21  | 1.86                     | 0.40              |
| 5:f:68:ARG:HD3    | 5:f:68:ARG:C     | 2.47                     | 0.40              |
| 6:g:97:ARG:NH2    | 6:g:112:LYS:HD2  | 2.36                     | 0.40              |
| 13:n:2:ARG:HA     | 13:n:5:LYS:CD    | 2.51                     | 0.40              |
| 13:n:31:HIS:O     | 13:n:32:GLU:HB3  | 2.22                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:p:93:LYS:HA   | 53:1:2848:G:H5''  | 2.03                     | 0.40              |
| 16:q:10:ARG:CZ   | 53:1:1216:G:C5'   | 2.99                     | 0.40              |
| 19:t:82:LYS:NZ   | 53:1:1339:G:OP1   | 2.54                     | 0.40              |
| 20:u:18:LYS:HD2  | 53:1:310:A:OP1    | 2.21                     | 0.40              |
| 32:H:174:LEU:HB2 | 52:3:1108:G:OP1   | 2.21                     | 0.40              |
| 36:L:86:VAL:HG13 | 36:L:86:VAL:O     | 2.21                     | 0.40              |
| 37:M:5:PRO:HG3   | 52:3:588:G:O3'    | 2.22                     | 0.40              |
| 37:M:79:ARG:HB2  | 52:3:878:A:OP1    | 2.21                     | 0.40              |
| 39:O:71:LEU:O    | 39:O:72:ARG:NH1   | 2.54                     | 0.40              |
| 40:P:33:ILE:O    | 40:P:33:ILE:HG23  | 2.21                     | 0.40              |
| 41:Q:98:ARG:NH1  | 41:Q:106:VAL:HG22 | 2.35                     | 0.40              |
| 47:W:43:ILE:HD12 | 47:W:43:ILE:N     | 2.37                     | 0.40              |
| 50:Z:13:VAL:HG13 | 50:Z:15:LEU:HD23  | 2.04                     | 0.40              |
| 51:a:67:HIS:HB2  | 51:a:188:ASN:HD21 | 1.87                     | 0.40              |
| 51:a:163:TYR:HB3 | 51:a:173:THR:HG22 | 2.03                     | 0.40              |
| 52:3:1490:U:H2'  | 52:3:1491:G:C8    | 2.56                     | 0.40              |
| 53:1:559:G:H2'   | 53:1:560:C:O4'    | 2.22                     | 0.40              |
| 53:1:657:U:H2'   | 53:1:658:U:C6     | 2.56                     | 0.40              |
| 53:1:876:C:H2'   | 53:1:877:A:O4'    | 2.21                     | 0.40              |
| 53:1:2030:A:N3   | 53:1:2499:C:H5''  | 2.37                     | 0.40              |
| 53:1:2098:U:H2'  | 53:1:2099:U:O4'   | 2.21                     | 0.40              |
| 53:1:2633:G:H5'  | 53:1:2811:G:O2'   | 2.22                     | 0.40              |
| 1:b:64:VAL:HG13  | 1:b:102:TYR:O     | 2.21                     | 0.40              |
| 4:e:134:GLN:N    | 4:e:134:GLN:OE1   | 2.55                     | 0.40              |
| 4:e:143:ASP:C    | 4:e:144:LYS:HD2   | 2.46                     | 0.40              |
| 7:h:117:LEU:HG   | 7:h:118:ILE:N     | 2.36                     | 0.40              |
| 9:j:7:LYS:O      | 9:j:11:VAL:HG23   | 2.21                     | 0.40              |
| 11:l:16:GLY:HA2  | 53:1:662:G:O3'    | 2.22                     | 0.40              |
| 11:l:85:VAL:HB   | 11:l:86:GLU:H     | 1.76                     | 0.40              |
| 13:n:115:LEU:C   | 13:n:117:ASP:N    | 2.80                     | 0.40              |
| 20:u:73:ASN:HB2  | 20:u:80:ASP:HB2   | 2.03                     | 0.40              |
| 28:D:1:MET:HB2   | 28:D:2:LYS:H      | 1.71                     | 0.40              |
| 29:E:39:ARG:O    | 29:E:43:LEU:HG    | 2.22                     | 0.40              |
| 32:H:126:ARG:N   | 32:H:126:ARG:HD3  | 2.37                     | 0.40              |
| 33:I:149:LYS:HG2 | 33:I:150:LYS:HG2  | 2.04                     | 0.40              |
| 37:M:12:ARG:NH2  | 52:3:826:C:H5'    | 2.36                     | 0.40              |
| 40:P:29:THR:OG1  | 40:P:46:ALA:HB2   | 2.22                     | 0.40              |
| 41:Q:31:GLY:O    | 41:Q:78:VAL:HG13  | 2.22                     | 0.40              |
| 43:S:2:LYS:HE2   | 52:3:1216:A:OP1   | 2.21                     | 0.40              |
| 43:S:33:VAL:HG12 | 43:S:33:VAL:O     | 2.21                     | 0.40              |
| 43:S:81:ILE:HD12 | 43:S:81:ILE:H     | 1.87                     | 0.40              |

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| Atom-1            | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-----------------|--------------------------|-------------------|
| 46:V:43:LEU:HD23  | 46:V:43:LEU:HA  | 1.90                     | 0.40              |
| 51:a:4:LEU:HD23   | 51:a:4:LEU:HA   | 1.96                     | 0.40              |
| 51:a:41:SER:HB3   | 53:1:2124:G:O2' | 2.22                     | 0.40              |
| 51:a:209:ILE:HG23 | 51:a:209:ILE:O  | 2.21                     | 0.40              |
| 52:3:125:U:H2'    | 52:3:126:G:C8   | 2.57                     | 0.40              |
| 52:3:243:A:H4'    | 52:3:244:U:H3'  | 2.04                     | 0.40              |
| 52:3:855:U:H2'    | 52:3:856:C:C6   | 2.57                     | 0.40              |
| 52:3:1414:U:H2'   | 52:3:1415:G:H8  | 1.87                     | 0.40              |
| 52:3:1496:C:H2'   | 52:3:1497:G:C8  | 2.57                     | 0.40              |
| 53:1:171:U:H2'    | 53:1:172:A:C8   | 2.56                     | 0.40              |
| 53:1:293:U:H2'    | 53:1:294:A:H5'' | 2.04                     | 0.40              |
| 53:1:329:G:O4'    | 53:1:477:A:H1'  | 2.21                     | 0.40              |
| 53:1:1601:G:C2'   | 53:1:1602:U:H5' | 2.52                     | 0.40              |
| 53:1:2512:C:H2'   | 53:1:2513:A:O4' | 2.22                     | 0.40              |
| 53:1:2873:A:O2'   | 53:1:2874:C:H5' | 2.21                     | 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     | 269/271 (99%) | 226 (84%) | 37 (14%) | 6 (2%)   | 5           | 29  |
| 2   | c     | 207/209 (99%) | 173 (84%) | 30 (14%) | 4 (2%)   | 6           | 32  |
| 3   | d     | 199/201 (99%) | 172 (86%) | 23 (12%) | 4 (2%)   | 6           | 31  |
| 4   | e     | 175/177 (99%) | 153 (87%) | 21 (12%) | 1 (1%)   | 21          | 58  |
| 5   | f     | 174/176 (99%) | 158 (91%) | 16 (9%)  | 0        | 100         | 100 |
| 6   | g     | 147/149 (99%) | 123 (84%) | 20 (14%) | 4 (3%)   | 4           | 25  |
| 7   | h     | 129/131 (98%) | 97 (75%)  | 27 (21%) | 5 (4%)   | 2           | 19  |
| 8   | i     | 139/141 (99%) | 118 (85%) | 17 (12%) | 4 (3%)   | 3           | 23  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 9   | j     | 140/142 (99%) | 122 (87%) | 15 (11%) | 3 (2%)   | 5           | 30  |
| 10  | k     | 120/122 (98%) | 101 (84%) | 16 (13%) | 3 (2%)   | 4           | 26  |
| 11  | l     | 141/143 (99%) | 122 (86%) | 16 (11%) | 3 (2%)   | 5           | 30  |
| 12  | m     | 134/136 (98%) | 112 (84%) | 18 (13%) | 4 (3%)   | 3           | 22  |
| 13  | n     | 118/120 (98%) | 97 (82%)  | 20 (17%) | 1 (1%)   | 16          | 52  |
| 14  | o     | 114/116 (98%) | 101 (89%) | 11 (10%) | 2 (2%)   | 6           | 33  |
| 15  | p     | 112/114 (98%) | 99 (88%)  | 11 (10%) | 2 (2%)   | 6           | 33  |
| 16  | q     | 115/117 (98%) | 103 (90%) | 10 (9%)  | 2 (2%)   | 7           | 35  |
| 17  | r     | 101/103 (98%) | 82 (81%)  | 17 (17%) | 2 (2%)   | 6           | 31  |
| 18  | s     | 108/110 (98%) | 90 (83%)  | 16 (15%) | 2 (2%)   | 6           | 32  |
| 19  | t     | 91/93 (98%)   | 81 (89%)  | 9 (10%)  | 1 (1%)   | 11          | 45  |
| 20  | u     | 100/102 (98%) | 86 (86%)  | 13 (13%) | 1 (1%)   | 12          | 47  |
| 21  | v     | 92/94 (98%)   | 80 (87%)  | 11 (12%) | 1 (1%)   | 11          | 45  |
| 22  | w     | 73/75 (97%)   | 62 (85%)  | 11 (15%) | 0        | 100         | 100 |
| 23  | x     | 75/77 (97%)   | 69 (92%)  | 4 (5%)   | 2 (3%)   | 4           | 25  |
| 24  | y     | 61/63 (97%)   | 58 (95%)  | 2 (3%)   | 1 (2%)   | 7           | 37  |
| 25  | z     | 56/58 (97%)   | 52 (93%)  | 3 (5%)   | 1 (2%)   | 6           | 33  |
| 26  | B     | 54/56 (96%)   | 46 (85%)  | 8 (15%)  | 0        | 100         | 100 |
| 27  | C     | 48/50 (96%)   | 44 (92%)  | 4 (8%)   | 0        | 100         | 100 |
| 28  | D     | 44/46 (96%)   | 38 (86%)  | 5 (11%)  | 1 (2%)   | 5           | 28  |
| 29  | E     | 62/64 (97%)   | 53 (86%)  | 7 (11%)  | 2 (3%)   | 3           | 21  |
| 30  | F     | 36/38 (95%)   | 27 (75%)  | 8 (22%)  | 1 (3%)   | 4           | 24  |
| 31  | G     | 223/225 (99%) | 201 (90%) | 22 (10%) | 0        | 100         | 100 |
| 32  | H     | 204/206 (99%) | 187 (92%) | 16 (8%)  | 1 (0%)   | 24          | 62  |
| 33  | I     | 203/205 (99%) | 179 (88%) | 19 (9%)  | 5 (2%)   | 4           | 26  |
| 34  | J     | 155/157 (99%) | 121 (78%) | 27 (17%) | 7 (4%)   | 2           | 17  |
| 35  | K     | 98/100 (98%)  | 79 (81%)  | 16 (16%) | 3 (3%)   | 3           | 22  |
| 36  | L     | 149/151 (99%) | 128 (86%) | 16 (11%) | 5 (3%)   | 3           | 21  |
| 37  | M     | 127/129 (98%) | 109 (86%) | 16 (13%) | 2 (2%)   | 7           | 37  |
| 38  | N     | 125/127 (98%) | 106 (85%) | 15 (12%) | 4 (3%)   | 3           | 21  |
| 39  | O     | 96/98 (98%)   | 74 (77%)  | 16 (17%) | 6 (6%)   | 1           | 13  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 40  | P     | 114/116 (98%)   | 94 (82%)   | 19 (17%)  | 1 (1%)   | 14          | 49  |
| 41  | Q     | 121/123 (98%)   | 99 (82%)   | 18 (15%)  | 4 (3%)   | 3           | 21  |
| 42  | R     | 112/114 (98%)   | 92 (82%)   | 15 (13%)  | 5 (4%)   | 2           | 17  |
| 43  | S     | 98/100 (98%)    | 81 (83%)   | 16 (16%)  | 1 (1%)   | 12          | 47  |
| 44  | T     | 86/88 (98%)     | 72 (84%)   | 10 (12%)  | 4 (5%)   | 2           | 16  |
| 45  | U     | 80/82 (98%)     | 68 (85%)   | 10 (12%)  | 2 (2%)   | 4           | 26  |
| 46  | V     | 78/80 (98%)     | 61 (78%)   | 14 (18%)  | 3 (4%)   | 2           | 19  |
| 47  | W     | 63/65 (97%)     | 58 (92%)   | 4 (6%)    | 1 (2%)   | 7           | 37  |
| 48  | X     | 77/79 (98%)     | 60 (78%)   | 16 (21%)  | 1 (1%)   | 9           | 41  |
| 49  | Y     | 83/85 (98%)     | 77 (93%)   | 4 (5%)    | 2 (2%)   | 4           | 27  |
| 50  | Z     | 63/65 (97%)     | 43 (68%)   | 13 (21%)  | 7 (11%)  | 0           | 6   |
| 51  | a     | 130/223 (58%)   | 117 (90%)  | 13 (10%)  | 0        | 100         | 100 |
| All | All   | 5919/6112 (97%) | 5051 (85%) | 741 (12%) | 127 (2%) | 8           | 30  |

All (127) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 58  | LYS  |
| 3   | d     | 83  | VAL  |
| 6   | g     | 9   | VAL  |
| 7   | h     | 108 | VAL  |
| 7   | h     | 118 | ILE  |
| 9   | j     | 81  | ILE  |
| 11  | l     | 85  | VAL  |
| 12  | m     | 58  | LYS  |
| 12  | m     | 59  | ARG  |
| 15  | p     | 113 | LEU  |
| 17  | r     | 54  | VAL  |
| 24  | y     | 24  | GLU  |
| 29  | E     | 17  | GLY  |
| 29  | E     | 31  | ILE  |
| 30  | F     | 37  | GLN  |
| 33  | I     | 4   | LEU  |
| 34  | J     | 93  | VAL  |
| 35  | K     | 95  | ALA  |
| 36  | L     | 56  | SER  |
| 41  | Q     | 24  | GLU  |
| 42  | R     | 4   | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | S     | 31  | SER  |
| 44  | T     | 46  | LYS  |
| 45  | U     | 79  | ASN  |
| 46  | V     | 49  | ASN  |
| 50  | Z     | 14  | ALA  |
| 1   | b     | 217 | PRO  |
| 2   | c     | 174 | SER  |
| 6   | g     | 41  | LYS  |
| 7   | h     | 80  | THR  |
| 7   | h     | 107 | GLU  |
| 8   | i     | 13  | ALA  |
| 9   | j     | 72  | LYS  |
| 9   | j     | 85  | LYS  |
| 10  | k     | 13  | ASN  |
| 11  | l     | 115 | GLU  |
| 12  | m     | 13  | HIS  |
| 12  | m     | 70  | ASP  |
| 16  | q     | 25  | GLY  |
| 19  | t     | 44  | LYS  |
| 23  | x     | 23  | ALA  |
| 38  | N     | 90  | ASP  |
| 39  | O     | 89  | ARG  |
| 41  | Q     | 77  | SER  |
| 42  | R     | 6   | ILE  |
| 42  | R     | 22  | TYR  |
| 44  | T     | 2   | LEU  |
| 50  | Z     | 12  | ASP  |
| 50  | Z     | 25  | ALA  |
| 50  | Z     | 34  | ARG  |
| 50  | Z     | 64  | ALA  |
| 1   | b     | 204 | LEU  |
| 1   | b     | 260 | LYS  |
| 3   | d     | 165 | HIS  |
| 7   | h     | 48  | ALA  |
| 8   | i     | 22  | PRO  |
| 10  | k     | 110 | GLU  |
| 13  | n     | 2   | ARG  |
| 16  | q     | 5   | ARG  |
| 18  | s     | 65  | ASP  |
| 21  | v     | 81  | PRO  |
| 32  | H     | 156 | LEU  |
| 33  | I     | 29  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | J     | 89  | THR  |
| 34  | J     | 90  | GLY  |
| 34  | J     | 122 | VAL  |
| 36  | L     | 129 | ASN  |
| 38  | N     | 8   | THR  |
| 38  | N     | 99  | LYS  |
| 39  | O     | 35  | GLN  |
| 42  | R     | 65  | GLU  |
| 46  | V     | 15  | LYS  |
| 46  | V     | 17  | GLU  |
| 49  | Y     | 6   | ALA  |
| 49  | Y     | 68  | LYS  |
| 50  | Z     | 9   | GLU  |
| 2   | c     | 31  | ALA  |
| 2   | c     | 86  | GLU  |
| 3   | d     | 184 | ASP  |
| 8   | i     | 11  | GLN  |
| 11  | l     | 88  | GLY  |
| 18  | s     | 64  | ALA  |
| 20  | u     | 97  | SER  |
| 33  | I     | 150 | LYS  |
| 34  | J     | 11  | GLN  |
| 35  | K     | 55  | HIS  |
| 35  | K     | 86  | ARG  |
| 38  | N     | 12  | LYS  |
| 39  | O     | 33  | GLY  |
| 44  | T     | 13  | GLU  |
| 47  | W     | 13  | THR  |
| 1   | b     | 209 | ALA  |
| 6   | g     | 12  | LEU  |
| 6   | g     | 89  | LYS  |
| 14  | o     | 34  | HIS  |
| 14  | o     | 114 | GLY  |
| 17  | r     | 44  | GLY  |
| 23  | x     | 43  | LYS  |
| 39  | O     | 42  | LEU  |
| 40  | P     | 92  | ARG  |
| 41  | Q     | 33  | CYS  |
| 42  | R     | 7   | ASN  |
| 44  | T     | 47  | LYS  |
| 45  | U     | 47  | GLU  |
| 50  | Z     | 10  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | e     | 175 | PRO  |
| 10  | k     | 72  | PRO  |
| 25  | z     | 11  | SER  |
| 28  | D     | 44  | VAL  |
| 34  | J     | 99  | SER  |
| 36  | L     | 18  | GLY  |
| 37  | M     | 125 | ILE  |
| 48  | X     | 29  | PRO  |
| 1   | b     | 7   | PRO  |
| 2   | c     | 143 | PRO  |
| 3   | d     | 177 | PRO  |
| 8   | i     | 21  | PRO  |
| 34  | J     | 97  | PRO  |
| 39  | O     | 41  | PRO  |
| 39  | O     | 43  | PRO  |
| 41  | Q     | 41  | PRO  |
| 33  | I     | 167 | PRO  |
| 36  | L     | 80  | GLY  |
| 37  | M     | 77  | VAL  |
| 33  | I     | 6   | PRO  |
| 15  | p     | 31  | VAL  |
| 36  | L     | 5   | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | b     | 216/216 (100%) | 212 (98%)  | 4 (2%)   | 50          | 66  |
| 2   | c     | 164/164 (100%) | 163 (99%)  | 1 (1%)   | 78          | 80  |
| 3   | d     | 165/165 (100%) | 163 (99%)  | 2 (1%)   | 63          | 73  |
| 4   | e     | 148/148 (100%) | 146 (99%)  | 2 (1%)   | 59          | 71  |
| 5   | f     | 137/137 (100%) | 137 (100%) | 0        | 100         | 100 |
| 6   | g     | 114/114 (100%) | 114 (100%) | 0        | 100         | 100 |
| 7   | h     | 100/100 (100%) | 99 (99%)   | 1 (1%)   | 68          | 76  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 8   | i     | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 9   | j     | 116/116 (100%) | 116 (100%) | 0        | 100         | 100 |
| 10  | k     | 103/103 (100%) | 102 (99%)  | 1 (1%)   | 68          | 76  |
| 11  | l     | 102/102 (100%) | 102 (100%) | 0        | 100         | 100 |
| 12  | m     | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 13  | n     | 100/100 (100%) | 97 (97%)   | 3 (3%)   | 36          | 57  |
| 14  | o     | 86/86 (100%)   | 85 (99%)   | 1 (1%)   | 63          | 73  |
| 15  | p     | 99/99 (100%)   | 98 (99%)   | 1 (1%)   | 68          | 76  |
| 16  | q     | 89/89 (100%)   | 88 (99%)   | 1 (1%)   | 65          | 74  |
| 17  | r     | 84/84 (100%)   | 83 (99%)   | 1 (1%)   | 63          | 73  |
| 18  | s     | 93/93 (100%)   | 91 (98%)   | 2 (2%)   | 45          | 64  |
| 19  | t     | 80/80 (100%)   | 80 (100%)  | 0        | 100         | 100 |
| 20  | u     | 83/83 (100%)   | 83 (100%)  | 0        | 100         | 100 |
| 21  | v     | 78/78 (100%)   | 77 (99%)   | 1 (1%)   | 61          | 72  |
| 22  | w     | 57/57 (100%)   | 56 (98%)   | 1 (2%)   | 51          | 67  |
| 23  | x     | 67/67 (100%)   | 65 (97%)   | 2 (3%)   | 36          | 57  |
| 24  | y     | 55/55 (100%)   | 55 (100%)  | 0        | 100         | 100 |
| 25  | z     | 48/48 (100%)   | 48 (100%)  | 0        | 100         | 100 |
| 26  | B     | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 27  | C     | 45/45 (100%)   | 44 (98%)   | 1 (2%)   | 45          | 64  |
| 28  | D     | 38/38 (100%)   | 38 (100%)  | 0        | 100         | 100 |
| 29  | E     | 51/51 (100%)   | 49 (96%)   | 2 (4%)   | 28          | 50  |
| 30  | F     | 34/34 (100%)   | 32 (94%)   | 2 (6%)   | 18          | 41  |
| 31  | G     | 186/186 (100%) | 185 (100%) | 1 (0%)   | 81          | 81  |
| 32  | H     | 170/170 (100%) | 167 (98%)  | 3 (2%)   | 51          | 67  |
| 33  | I     | 172/172 (100%) | 171 (99%)  | 1 (1%)   | 78          | 80  |
| 34  | J     | 119/119 (100%) | 119 (100%) | 0        | 100         | 100 |
| 35  | K     | 87/87 (100%)   | 86 (99%)   | 1 (1%)   | 65          | 74  |
| 36  | L     | 124/124 (100%) | 122 (98%)  | 2 (2%)   | 55          | 69  |
| 37  | M     | 104/104 (100%) | 100 (96%)  | 4 (4%)   | 29          | 51  |
| 38  | N     | 105/105 (100%) | 105 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 39  | O     | 86/86 (100%)    | 85 (99%)   | 1 (1%)   | 63          | 73  |
| 40  | P     | 89/89 (100%)    | 89 (100%)  | 0        | 100         | 100 |
| 41  | Q     | 103/103 (100%)  | 103 (100%) | 0        | 100         | 100 |
| 42  | R     | 92/92 (100%)    | 91 (99%)   | 1 (1%)   | 65          | 74  |
| 43  | S     | 83/83 (100%)    | 82 (99%)   | 1 (1%)   | 63          | 73  |
| 44  | T     | 76/76 (100%)    | 74 (97%)   | 2 (3%)   | 40          | 60  |
| 45  | U     | 65/65 (100%)    | 64 (98%)   | 1 (2%)   | 57          | 70  |
| 46  | V     | 74/74 (100%)    | 74 (100%)  | 0        | 100         | 100 |
| 47  | W     | 56/56 (100%)    | 56 (100%)  | 0        | 100         | 100 |
| 48  | X     | 70/70 (100%)    | 69 (99%)   | 1 (1%)   | 59          | 71  |
| 49  | Y     | 65/65 (100%)    | 65 (100%)  | 0        | 100         | 100 |
| 50  | Z     | 55/55 (100%)    | 55 (100%)  | 0        | 100         | 100 |
| 51  | a     | 110/174 (63%)   | 108 (98%)  | 2 (2%)   | 51          | 67  |
| All | All   | 4908/4972 (99%) | 4858 (99%) | 50 (1%)  | 65          | 76  |

All (50) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 85  | ASN  |
| 1   | b     | 119 | VAL  |
| 1   | b     | 140 | VAL  |
| 1   | b     | 181 | ARG  |
| 2   | c     | 201 | LEU  |
| 3   | d     | 91  | ASP  |
| 3   | d     | 154 | ASP  |
| 4   | e     | 65  | LEU  |
| 4   | e     | 158 | THR  |
| 7   | h     | 118 | ILE  |
| 10  | k     | 41  | ILE  |
| 13  | n     | 13  | ASN  |
| 13  | n     | 54  | LEU  |
| 13  | n     | 70  | THR  |
| 14  | o     | 81  | ARG  |
| 15  | p     | 109 | ILE  |
| 16  | q     | 61  | ILE  |
| 17  | r     | 22  | LEU  |
| 18  | s     | 34  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | s     | 52  | GLU  |
| 21  | v     | 70  | ILE  |
| 22  | w     | 42  | HIS  |
| 23  | x     | 16  | ASN  |
| 23  | x     | 29  | LEU  |
| 27  | C     | 21  | THR  |
| 29  | E     | 32  | LEU  |
| 29  | E     | 61  | LEU  |
| 30  | F     | 2   | LYS  |
| 30  | F     | 17  | VAL  |
| 31  | G     | 26  | MET  |
| 32  | H     | 13  | ILE  |
| 32  | H     | 123 | LEU  |
| 32  | H     | 156 | LEU  |
| 33  | I     | 54  | LEU  |
| 35  | K     | 39  | LEU  |
| 36  | L     | 115 | MET  |
| 36  | L     | 128 | GLU  |
| 37  | M     | 10  | LEU  |
| 37  | M     | 63  | LYS  |
| 37  | M     | 98  | LEU  |
| 37  | M     | 127 | TYR  |
| 39  | O     | 83  | THR  |
| 42  | R     | 101 | THR  |
| 43  | S     | 26  | LEU  |
| 44  | T     | 23  | SER  |
| 44  | T     | 80  | LEU  |
| 45  | U     | 19  | VAL  |
| 48  | X     | 23  | GLU  |
| 51  | a     | 170 | ILE  |
| 51  | a     | 222 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 36  | ASN  |
| 1   | b     | 45  | ASN  |
| 1   | b     | 85  | ASN  |
| 1   | b     | 116 | GLN  |
| 1   | b     | 152 | GLN  |
| 1   | b     | 162 | GLN  |
| 1   | b     | 196 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 199 | HIS  |
| 1   | b     | 242 | HIS  |
| 1   | b     | 259 | ASN  |
| 2   | c     | 32  | ASN  |
| 2   | c     | 36  | GLN  |
| 2   | c     | 49  | GLN  |
| 2   | c     | 149 | ASN  |
| 2   | c     | 150 | GLN  |
| 3   | d     | 9   | GLN  |
| 3   | d     | 94  | GLN  |
| 3   | d     | 97  | ASN  |
| 4   | e     | 20  | ASN  |
| 4   | e     | 26  | GLN  |
| 5   | f     | 37  | ASN  |
| 5   | f     | 44  | HIS  |
| 5   | f     | 63  | GLN  |
| 6   | g     | 11  | ASN  |
| 6   | g     | 33  | GLN  |
| 6   | g     | 66  | ASN  |
| 6   | g     | 145 | ASN  |
| 7   | h     | 6   | GLN  |
| 7   | h     | 103 | ASN  |
| 8   | i     | 18  | ASN  |
| 8   | i     | 29  | GLN  |
| 8   | i     | 33  | ASN  |
| 8   | i     | 42  | ASN  |
| 9   | j     | 135 | GLN  |
| 10  | k     | 3   | GLN  |
| 10  | k     | 88  | ASN  |
| 11  | l     | 38  | GLN  |
| 12  | m     | 3   | GLN  |
| 12  | m     | 13  | HIS  |
| 12  | m     | 60  | GLN  |
| 12  | m     | 88  | ASN  |
| 13  | n     | 18  | GLN  |
| 13  | n     | 23  | ASN  |
| 13  | n     | 62  | ASN  |
| 13  | n     | 73  | ASN  |
| 14  | o     | 116 | GLN  |
| 15  | p     | 11  | GLN  |
| 15  | p     | 55  | HIS  |
| 16  | q     | 19  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | q     | 43  | GLN  |
| 16  | q     | 55  | GLN  |
| 16  | q     | 58  | GLN  |
| 16  | q     | 65  | ASN  |
| 16  | q     | 71  | ASN  |
| 17  | r     | 12  | HIS  |
| 18  | s     | 7   | HIS  |
| 18  | s     | 9   | HIS  |
| 18  | s     | 40  | ASN  |
| 19  | t     | 15  | HIS  |
| 20  | u     | 26  | ASN  |
| 20  | u     | 65  | GLN  |
| 20  | u     | 73  | ASN  |
| 21  | v     | 49  | ASN  |
| 21  | v     | 51  | GLN  |
| 21  | v     | 75  | GLN  |
| 21  | v     | 78  | GLN  |
| 21  | v     | 80  | HIS  |
| 22  | w     | 8   | ASN  |
| 22  | w     | 42  | HIS  |
| 23  | x     | 16  | ASN  |
| 23  | x     | 31  | ASN  |
| 24  | y     | 41  | HIS  |
| 25  | z     | 48  | ASN  |
| 26  | B     | 5   | ASN  |
| 26  | B     | 18  | HIS  |
| 31  | G     | 121 | GLN  |
| 32  | H     | 2   | GLN  |
| 32  | H     | 18  | ASN  |
| 32  | H     | 31  | ASN  |
| 32  | H     | 68  | HIS  |
| 32  | H     | 139 | ASN  |
| 33  | I     | 88  | ASN  |
| 33  | I     | 197 | HIS  |
| 34  | J     | 131 | ASN  |
| 35  | K     | 52  | ASN  |
| 35  | K     | 58  | HIS  |
| 35  | K     | 63  | ASN  |
| 35  | K     | 81  | ASN  |
| 35  | K     | 94  | HIS  |
| 36  | L     | 27  | ASN  |
| 36  | L     | 67  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | L     | 121 | ASN  |
| 36  | L     | 129 | ASN  |
| 37  | M     | 3   | GLN  |
| 37  | M     | 20  | ASN  |
| 37  | M     | 66  | GLN  |
| 38  | N     | 3   | ASN  |
| 38  | N     | 24  | ASN  |
| 39  | O     | 64  | GLN  |
| 39  | O     | 99  | GLN  |
| 40  | P     | 39  | ASN  |
| 40  | P     | 63  | GLN  |
| 40  | P     | 100 | ASN  |
| 40  | P     | 118 | ASN  |
| 41  | Q     | 58  | ASN  |
| 42  | R     | 7   | ASN  |
| 42  | R     | 99  | GLN  |
| 43  | S     | 59  | GLN  |
| 44  | T     | 34  | GLN  |
| 44  | T     | 36  | ASN  |
| 44  | T     | 41  | HIS  |
| 45  | U     | 18  | GLN  |
| 49  | Y     | 20  | ASN  |
| 49  | Y     | 54  | GLN  |
| 49  | Y     | 81  | GLN  |
| 49  | Y     | 83  | ASN  |
| 51  | a     | 24  | ASN  |
| 51  | a     | 160 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 52  | 3     | 1538/1539 (99%) | 139 (9%)          | 3 (0%)          |
| 53  | 1     | 2902/2903 (99%) | 323 (11%)         | 8 (0%)          |
| 54  | 2     | 119/120 (99%)   | 11 (9%)           | 1 (0%)          |
| 55  | 5     | 76/77 (98%)     | 12 (15%)          | 0               |
| 55  | 6     | 76/77 (98%)     | 8 (10%)           | 0               |
| 56  | 4     | 17/18 (94%)     | 2 (11%)           | 0               |
| 57  | 7     | 72/76 (94%)     | 11 (15%)          | 0               |
| All | All   | 4800/4810 (99%) | 506 (10%)         | 12 (0%)         |

All (506) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | 3     | 6   | G    |
| 52  | 3     | 7   | A    |
| 52  | 3     | 9   | G    |
| 52  | 3     | 22  | G    |
| 52  | 3     | 31  | G    |
| 52  | 3     | 32  | A    |
| 52  | 3     | 39  | G    |
| 52  | 3     | 48  | C    |
| 52  | 3     | 51  | A    |
| 52  | 3     | 71  | A    |
| 52  | 3     | 85  | U    |
| 52  | 3     | 87  | C    |
| 52  | 3     | 130 | A    |
| 52  | 3     | 144 | G    |
| 52  | 3     | 183 | C    |
| 52  | 3     | 184 | G    |
| 52  | 3     | 197 | A    |
| 52  | 3     | 209 | U    |
| 52  | 3     | 210 | C    |
| 52  | 3     | 226 | G    |
| 52  | 3     | 247 | G    |
| 52  | 3     | 251 | G    |
| 52  | 3     | 266 | G    |
| 52  | 3     | 267 | C    |
| 52  | 3     | 281 | G    |
| 52  | 3     | 289 | G    |
| 52  | 3     | 345 | C    |
| 52  | 3     | 346 | G    |
| 52  | 3     | 352 | C    |
| 52  | 3     | 367 | U    |
| 52  | 3     | 372 | C    |
| 52  | 3     | 411 | A    |
| 52  | 3     | 412 | A    |
| 52  | 3     | 413 | G    |
| 52  | 3     | 429 | U    |
| 52  | 3     | 467 | U    |
| 52  | 3     | 485 | U    |
| 52  | 3     | 486 | U    |
| 52  | 3     | 497 | G    |
| 52  | 3     | 518 | C    |
| 52  | 3     | 532 | A    |
| 52  | 3     | 533 | A    |
| 52  | 3     | 547 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 52  | 3     | 561  | U    |
| 52  | 3     | 572  | A    |
| 52  | 3     | 573  | A    |
| 52  | 3     | 575  | G    |
| 52  | 3     | 576  | C    |
| 52  | 3     | 577  | G    |
| 52  | 3     | 633  | G    |
| 52  | 3     | 653  | U    |
| 52  | 3     | 665  | A    |
| 52  | 3     | 687  | A    |
| 52  | 3     | 688  | G    |
| 52  | 3     | 702  | A    |
| 52  | 3     | 703  | G    |
| 52  | 3     | 724  | G    |
| 52  | 3     | 755  | G    |
| 52  | 3     | 777  | A    |
| 52  | 3     | 815  | A    |
| 52  | 3     | 817  | C    |
| 52  | 3     | 818  | G    |
| 52  | 3     | 819  | A    |
| 52  | 3     | 821  | G    |
| 52  | 3     | 843  | U    |
| 52  | 3     | 844  | G    |
| 52  | 3     | 846  | G    |
| 52  | 3     | 871  | U    |
| 52  | 3     | 873  | A    |
| 52  | 3     | 890  | G    |
| 52  | 3     | 902  | G    |
| 52  | 3     | 934  | C    |
| 52  | 3     | 935  | A    |
| 52  | 3     | 960  | U    |
| 52  | 3     | 961  | U    |
| 52  | 3     | 966  | G    |
| 52  | 3     | 969  | A    |
| 52  | 3     | 975  | A    |
| 52  | 3     | 976  | G    |
| 52  | 3     | 977  | A    |
| 52  | 3     | 992  | U    |
| 52  | 3     | 993  | G    |
| 52  | 3     | 1004 | A    |
| 52  | 3     | 1028 | C    |
| 52  | 3     | 1030 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 52  | 3     | 1031 | C    |
| 52  | 3     | 1033 | G    |
| 52  | 3     | 1034 | G    |
| 52  | 3     | 1094 | G    |
| 52  | 3     | 1101 | A    |
| 52  | 3     | 1136 | C    |
| 52  | 3     | 1137 | C    |
| 52  | 3     | 1138 | G    |
| 52  | 3     | 1139 | G    |
| 52  | 3     | 1159 | U    |
| 52  | 3     | 1168 | U    |
| 52  | 3     | 1182 | G    |
| 52  | 3     | 1184 | G    |
| 52  | 3     | 1191 | A    |
| 52  | 3     | 1196 | A    |
| 52  | 3     | 1198 | G    |
| 52  | 3     | 1201 | A    |
| 52  | 3     | 1202 | U    |
| 52  | 3     | 1213 | A    |
| 52  | 3     | 1225 | A    |
| 52  | 3     | 1238 | A    |
| 52  | 3     | 1240 | U    |
| 52  | 3     | 1241 | G    |
| 52  | 3     | 1258 | G    |
| 52  | 3     | 1260 | G    |
| 52  | 3     | 1275 | A    |
| 52  | 3     | 1278 | G    |
| 52  | 3     | 1280 | A    |
| 52  | 3     | 1282 | C    |
| 52  | 3     | 1286 | U    |
| 52  | 3     | 1287 | A    |
| 52  | 3     | 1300 | G    |
| 52  | 3     | 1302 | C    |
| 52  | 3     | 1317 | C    |
| 52  | 3     | 1320 | C    |
| 52  | 3     | 1346 | A    |
| 52  | 3     | 1347 | G    |
| 52  | 3     | 1363 | A    |
| 52  | 3     | 1364 | U    |
| 52  | 3     | 1378 | C    |
| 52  | 3     | 1381 | U    |
| 52  | 3     | 1395 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 52  | 3     | 1446 | A    |
| 52  | 3     | 1448 | C    |
| 52  | 3     | 1451 | U    |
| 52  | 3     | 1452 | C    |
| 52  | 3     | 1492 | A    |
| 52  | 3     | 1493 | A    |
| 52  | 3     | 1503 | A    |
| 52  | 3     | 1506 | U    |
| 52  | 3     | 1517 | G    |
| 52  | 3     | 1529 | G    |
| 52  | 3     | 1530 | G    |
| 52  | 3     | 1540 | U    |
| 53  | 1     | 10   | A    |
| 53  | 1     | 12   | U    |
| 53  | 1     | 34   | U    |
| 53  | 1     | 35   | G    |
| 53  | 1     | 46   | G    |
| 53  | 1     | 49   | A    |
| 53  | 1     | 50   | U    |
| 53  | 1     | 51   | G    |
| 53  | 1     | 63   | A    |
| 53  | 1     | 71   | A    |
| 53  | 1     | 74   | A    |
| 53  | 1     | 75   | G    |
| 53  | 1     | 120  | U    |
| 53  | 1     | 125  | A    |
| 53  | 1     | 138  | U    |
| 53  | 1     | 139  | U    |
| 53  | 1     | 140  | C    |
| 53  | 1     | 141  | G    |
| 53  | 1     | 142  | A    |
| 53  | 1     | 162  | U    |
| 53  | 1     | 163  | C    |
| 53  | 1     | 181  | A    |
| 53  | 1     | 196  | A    |
| 53  | 1     | 216  | A    |
| 53  | 1     | 221  | A    |
| 53  | 1     | 222  | A    |
| 53  | 1     | 229  | C    |
| 53  | 1     | 248  | G    |
| 53  | 1     | 249  | C    |
| 53  | 1     | 255  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 1     | 265 | A    |
| 53  | 1     | 266 | G    |
| 53  | 1     | 276 | U    |
| 53  | 1     | 281 | C    |
| 53  | 1     | 294 | A    |
| 53  | 1     | 301 | G    |
| 53  | 1     | 311 | A    |
| 53  | 1     | 323 | C    |
| 53  | 1     | 324 | A    |
| 53  | 1     | 329 | G    |
| 53  | 1     | 330 | A    |
| 53  | 1     | 371 | A    |
| 53  | 1     | 372 | G    |
| 53  | 1     | 386 | G    |
| 53  | 1     | 387 | U    |
| 53  | 1     | 404 | A    |
| 53  | 1     | 406 | G    |
| 53  | 1     | 411 | G    |
| 53  | 1     | 424 | G    |
| 53  | 1     | 451 | U    |
| 53  | 1     | 457 | A    |
| 53  | 1     | 458 | G    |
| 53  | 1     | 481 | G    |
| 53  | 1     | 491 | G    |
| 53  | 1     | 504 | A    |
| 53  | 1     | 505 | A    |
| 53  | 1     | 529 | A    |
| 53  | 1     | 530 | G    |
| 53  | 1     | 531 | C    |
| 53  | 1     | 532 | A    |
| 53  | 1     | 543 | G    |
| 53  | 1     | 545 | U    |
| 53  | 1     | 563 | A    |
| 53  | 1     | 572 | A    |
| 53  | 1     | 573 | U    |
| 53  | 1     | 588 | U    |
| 53  | 1     | 603 | A    |
| 53  | 1     | 614 | A    |
| 53  | 1     | 616 | A    |
| 53  | 1     | 627 | A    |
| 53  | 1     | 637 | A    |
| 53  | 1     | 646 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 654  | A    |
| 53  | 1     | 669  | G    |
| 53  | 1     | 686  | U    |
| 53  | 1     | 687  | C    |
| 53  | 1     | 695  | G    |
| 53  | 1     | 730  | A    |
| 53  | 1     | 747  | C    |
| 53  | 1     | 752  | A    |
| 53  | 1     | 764  | A    |
| 53  | 1     | 776  | G    |
| 53  | 1     | 782  | A    |
| 53  | 1     | 784  | G    |
| 53  | 1     | 785  | G    |
| 53  | 1     | 805  | G    |
| 53  | 1     | 812  | C    |
| 53  | 1     | 819  | A    |
| 53  | 1     | 822  | G    |
| 53  | 1     | 827  | U    |
| 53  | 1     | 828  | U    |
| 53  | 1     | 830  | G    |
| 53  | 1     | 845  | A    |
| 53  | 1     | 846  | U    |
| 53  | 1     | 847  | U    |
| 53  | 1     | 860  | U    |
| 53  | 1     | 878  | A    |
| 53  | 1     | 886  | A    |
| 53  | 1     | 887  | U    |
| 53  | 1     | 888  | C    |
| 53  | 1     | 896  | A    |
| 53  | 1     | 897  | C    |
| 53  | 1     | 910  | A    |
| 53  | 1     | 932  | U    |
| 53  | 1     | 941  | A    |
| 53  | 1     | 946  | C    |
| 53  | 1     | 961  | C    |
| 53  | 1     | 974  | G    |
| 53  | 1     | 975  | A    |
| 53  | 1     | 983  | A    |
| 53  | 1     | 995  | C    |
| 53  | 1     | 996  | A    |
| 53  | 1     | 1009 | A    |
| 53  | 1     | 1012 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 1013 | C    |
| 53  | 1     | 1021 | A    |
| 53  | 1     | 1022 | G    |
| 53  | 1     | 1026 | G    |
| 53  | 1     | 1033 | U    |
| 53  | 1     | 1045 | C    |
| 53  | 1     | 1046 | A    |
| 53  | 1     | 1047 | G    |
| 53  | 1     | 1054 | A    |
| 53  | 1     | 1060 | U    |
| 53  | 1     | 1062 | G    |
| 53  | 1     | 1066 | U    |
| 53  | 1     | 1070 | A    |
| 53  | 1     | 1071 | G    |
| 53  | 1     | 1079 | C    |
| 53  | 1     | 1084 | A    |
| 53  | 1     | 1088 | A    |
| 53  | 1     | 1104 | C    |
| 53  | 1     | 1106 | G    |
| 53  | 1     | 1111 | A    |
| 53  | 1     | 1131 | G    |
| 53  | 1     | 1132 | U    |
| 53  | 1     | 1133 | A    |
| 53  | 1     | 1135 | C    |
| 53  | 1     | 1143 | A    |
| 53  | 1     | 1157 | G    |
| 53  | 1     | 1175 | A    |
| 53  | 1     | 1177 | G    |
| 53  | 1     | 1178 | C    |
| 53  | 1     | 1180 | U    |
| 53  | 1     | 1212 | G    |
| 53  | 1     | 1251 | C    |
| 53  | 1     | 1253 | A    |
| 53  | 1     | 1256 | G    |
| 53  | 1     | 1271 | G    |
| 53  | 1     | 1272 | A    |
| 53  | 1     | 1275 | A    |
| 53  | 1     | 1289 | C    |
| 53  | 1     | 1300 | G    |
| 53  | 1     | 1301 | A    |
| 53  | 1     | 1302 | A    |
| 53  | 1     | 1329 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 1330 | C    |
| 53  | 1     | 1332 | G    |
| 53  | 1     | 1345 | C    |
| 53  | 1     | 1365 | A    |
| 53  | 1     | 1379 | U    |
| 53  | 1     | 1383 | A    |
| 53  | 1     | 1398 | C    |
| 53  | 1     | 1416 | G    |
| 53  | 1     | 1419 | A    |
| 53  | 1     | 1420 | A    |
| 53  | 1     | 1454 | C    |
| 53  | 1     | 1461 | C    |
| 53  | 1     | 1482 | G    |
| 53  | 1     | 1490 | A    |
| 53  | 1     | 1491 | G    |
| 53  | 1     | 1493 | C    |
| 53  | 1     | 1498 | C    |
| 53  | 1     | 1515 | A    |
| 53  | 1     | 1524 | G    |
| 53  | 1     | 1535 | A    |
| 53  | 1     | 1536 | C    |
| 53  | 1     | 1537 | G    |
| 53  | 1     | 1555 | G    |
| 53  | 1     | 1559 | U    |
| 53  | 1     | 1560 | G    |
| 53  | 1     | 1569 | A    |
| 53  | 1     | 1581 | G    |
| 53  | 1     | 1585 | C    |
| 53  | 1     | 1608 | A    |
| 53  | 1     | 1611 | C    |
| 53  | 1     | 1616 | A    |
| 53  | 1     | 1647 | U    |
| 53  | 1     | 1648 | U    |
| 53  | 1     | 1654 | A    |
| 53  | 1     | 1674 | G    |
| 53  | 1     | 1699 | G    |
| 53  | 1     | 1715 | G    |
| 53  | 1     | 1729 | U    |
| 53  | 1     | 1730 | C    |
| 53  | 1     | 1732 | C    |
| 53  | 1     | 1738 | G    |
| 53  | 1     | 1758 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 1764 | C    |
| 53  | 1     | 1773 | A    |
| 53  | 1     | 1780 | A    |
| 53  | 1     | 1800 | C    |
| 53  | 1     | 1801 | A    |
| 53  | 1     | 1808 | A    |
| 53  | 1     | 1816 | C    |
| 53  | 1     | 1871 | A    |
| 53  | 1     | 1901 | A    |
| 53  | 1     | 1906 | G    |
| 53  | 1     | 1907 | G    |
| 53  | 1     | 1913 | A    |
| 53  | 1     | 1929 | G    |
| 53  | 1     | 1930 | G    |
| 53  | 1     | 1937 | A    |
| 53  | 1     | 1938 | A    |
| 53  | 1     | 1955 | U    |
| 53  | 1     | 1963 | U    |
| 53  | 1     | 1967 | C    |
| 53  | 1     | 1970 | A    |
| 53  | 1     | 1972 | G    |
| 53  | 1     | 1993 | U    |
| 53  | 1     | 1997 | C    |
| 53  | 1     | 2022 | U    |
| 53  | 1     | 2023 | C    |
| 53  | 1     | 2030 | A    |
| 53  | 1     | 2031 | A    |
| 53  | 1     | 2036 | C    |
| 53  | 1     | 2043 | C    |
| 53  | 1     | 2049 | G    |
| 53  | 1     | 2055 | C    |
| 53  | 1     | 2056 | G    |
| 53  | 1     | 2060 | A    |
| 53  | 1     | 2061 | G    |
| 53  | 1     | 2062 | A    |
| 53  | 1     | 2069 | G    |
| 53  | 1     | 2072 | C    |
| 53  | 1     | 2093 | G    |
| 53  | 1     | 2110 | G    |
| 53  | 1     | 2111 | U    |
| 53  | 1     | 2112 | G    |
| 53  | 1     | 2113 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 2118 | U    |
| 53  | 1     | 2119 | A    |
| 53  | 1     | 2131 | U    |
| 53  | 1     | 2132 | U    |
| 53  | 1     | 2133 | G    |
| 53  | 1     | 2145 | C    |
| 53  | 1     | 2147 | A    |
| 53  | 1     | 2162 | G    |
| 53  | 1     | 2164 | C    |
| 53  | 1     | 2172 | U    |
| 53  | 1     | 2173 | A    |
| 53  | 1     | 2198 | A    |
| 53  | 1     | 2203 | U    |
| 53  | 1     | 2204 | G    |
| 53  | 1     | 2225 | A    |
| 53  | 1     | 2278 | A    |
| 53  | 1     | 2283 | C    |
| 53  | 1     | 2287 | A    |
| 53  | 1     | 2297 | A    |
| 53  | 1     | 2305 | U    |
| 53  | 1     | 2309 | A    |
| 53  | 1     | 2325 | G    |
| 53  | 1     | 2327 | A    |
| 53  | 1     | 2334 | U    |
| 53  | 1     | 2335 | A    |
| 53  | 1     | 2350 | C    |
| 53  | 1     | 2383 | G    |
| 53  | 1     | 2385 | C    |
| 53  | 1     | 2392 | A    |
| 53  | 1     | 2402 | U    |
| 53  | 1     | 2407 | A    |
| 53  | 1     | 2423 | U    |
| 53  | 1     | 2424 | C    |
| 53  | 1     | 2427 | C    |
| 53  | 1     | 2429 | G    |
| 53  | 1     | 2430 | A    |
| 53  | 1     | 2435 | A    |
| 53  | 1     | 2441 | U    |
| 53  | 1     | 2448 | A    |
| 53  | 1     | 2476 | A    |
| 53  | 1     | 2491 | U    |
| 53  | 1     | 2498 | C    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 2503 | A    |
| 53  | 1     | 2504 | U    |
| 53  | 1     | 2505 | G    |
| 53  | 1     | 2518 | A    |
| 53  | 1     | 2547 | A    |
| 53  | 1     | 2554 | U    |
| 53  | 1     | 2566 | A    |
| 53  | 1     | 2567 | G    |
| 53  | 1     | 2572 | A    |
| 53  | 1     | 2602 | A    |
| 53  | 1     | 2603 | G    |
| 53  | 1     | 2609 | U    |
| 53  | 1     | 2613 | U    |
| 53  | 1     | 2629 | U    |
| 53  | 1     | 2646 | C    |
| 53  | 1     | 2655 | G    |
| 53  | 1     | 2682 | A    |
| 53  | 1     | 2689 | U    |
| 53  | 1     | 2690 | U    |
| 53  | 1     | 2714 | G    |
| 53  | 1     | 2744 | G    |
| 53  | 1     | 2748 | A    |
| 53  | 1     | 2751 | G    |
| 53  | 1     | 2757 | A    |
| 53  | 1     | 2764 | A    |
| 53  | 1     | 2765 | A    |
| 53  | 1     | 2778 | A    |
| 53  | 1     | 2779 | U    |
| 53  | 1     | 2791 | G    |
| 53  | 1     | 2794 | C    |
| 53  | 1     | 2797 | U    |
| 53  | 1     | 2800 | A    |
| 53  | 1     | 2809 | A    |
| 53  | 1     | 2820 | A    |
| 53  | 1     | 2821 | A    |
| 53  | 1     | 2833 | U    |
| 53  | 1     | 2867 | G    |
| 53  | 1     | 2868 | A    |
| 53  | 1     | 2872 | A    |
| 53  | 1     | 2880 | C    |
| 53  | 1     | 2884 | U    |
| 54  | 2     | 4    | C    |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | 2     | 12  | C    |
| 54  | 2     | 13  | G    |
| 54  | 2     | 24  | G    |
| 54  | 2     | 35  | C    |
| 54  | 2     | 44  | G    |
| 54  | 2     | 67  | G    |
| 54  | 2     | 89  | U    |
| 54  | 2     | 90  | C    |
| 54  | 2     | 108 | A    |
| 54  | 2     | 109 | A    |
| 55  | 5     | 8   | U    |
| 55  | 5     | 9   | G    |
| 55  | 5     | 14  | A    |
| 55  | 5     | 18  | G    |
| 55  | 5     | 19  | G    |
| 55  | 5     | 20  | U    |
| 55  | 5     | 47  | U    |
| 55  | 5     | 48  | C    |
| 55  | 5     | 56  | C    |
| 55  | 5     | 58  | A    |
| 55  | 5     | 61  | C    |
| 55  | 5     | 76  | A    |
| 55  | 6     | 6   | G    |
| 55  | 6     | 16  | C    |
| 55  | 6     | 18  | G    |
| 55  | 6     | 19  | G    |
| 55  | 6     | 20  | U    |
| 55  | 6     | 47  | U    |
| 55  | 6     | 48  | C    |
| 55  | 6     | 61  | C    |
| 56  | 4     | 12  | A    |
| 56  | 4     | 13  | A    |
| 57  | 7     | 8   | U    |
| 57  | 7     | 17  | C    |
| 57  | 7     | 21  | A    |
| 57  | 7     | 45  | U    |
| 57  | 7     | 46  | G    |
| 57  | 7     | 47  | U    |
| 57  | 7     | 48  | C    |
| 57  | 7     | 49  | C    |
| 57  | 7     | 59  | U    |
| 57  | 7     | 61  | C    |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | 7     | 72  | C    |

All (12) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 52  | 3     | 70   | U    |
| 52  | 3     | 1190 | G    |
| 52  | 3     | 1201 | A    |
| 53  | 1     | 490  | C    |
| 53  | 1     | 859  | G    |
| 53  | 1     | 1020 | A    |
| 53  | 1     | 1130 | U    |
| 53  | 1     | 2286 | G    |
| 53  | 1     | 2296 | U    |
| 53  | 1     | 2326 | C    |
| 53  | 1     | 2391 | G    |
| 54  | 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](#)

1 ligand is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 58  | FME  | 5     | 101 | 55   | 8,9,10       | 0.81 | 0           | 8,9,11      | 0.70 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 58  | FME  | 5     | 101 | 55   | -       | 1/7/9/11 | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 58  | 5     | 101 | FME  | O1-CN-N-CA |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 58  | 5     | 101 | FME  | 1       | 0            |

## 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.

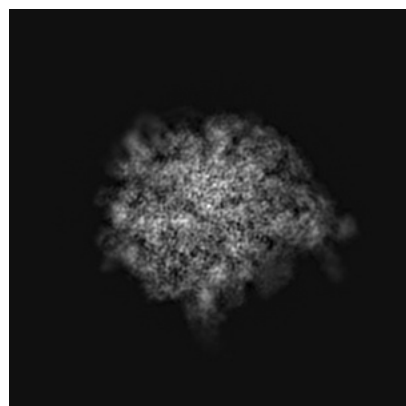
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21636. These allow visual inspection of the internal detail of the map and identification of artifacts.

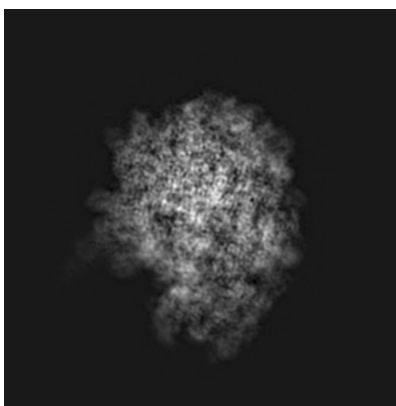
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

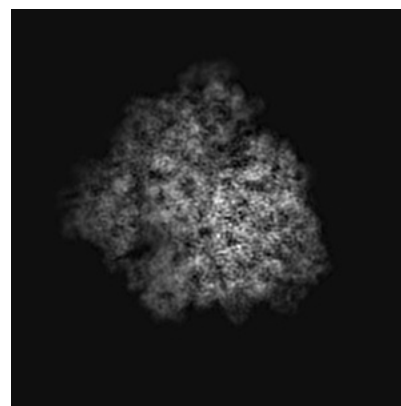
#### 6.1.1 Primary map



X

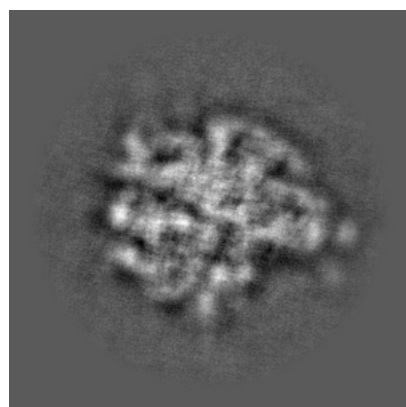


Y

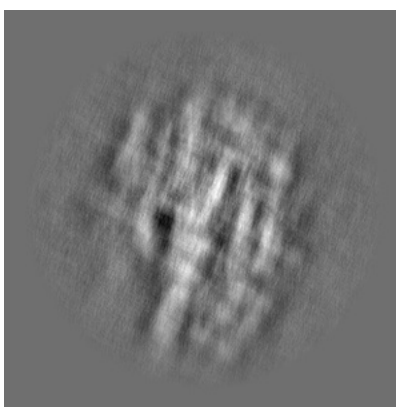


Z

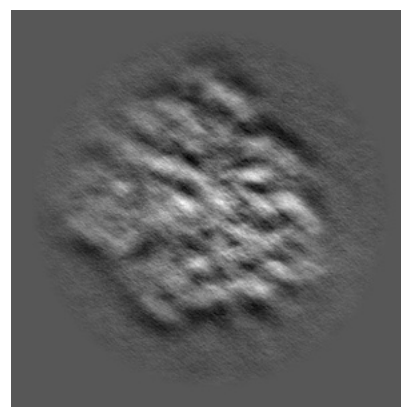
#### 6.1.2 Raw map



X



Y

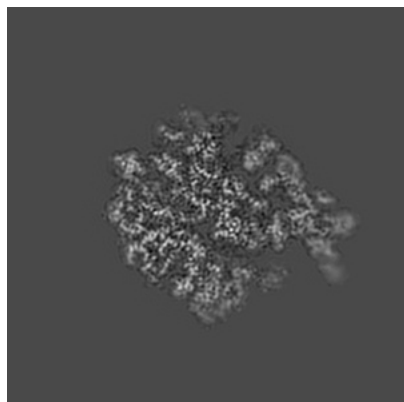


Z

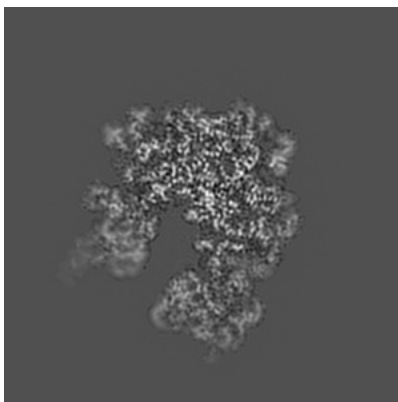
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

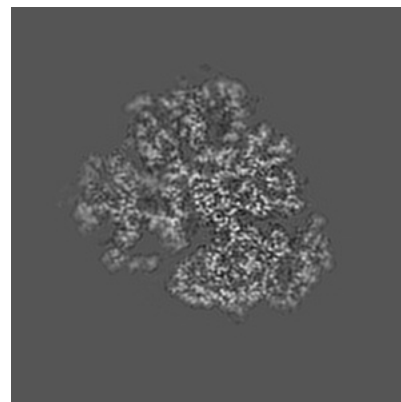
### 6.2.1 Primary map



X Index: 144

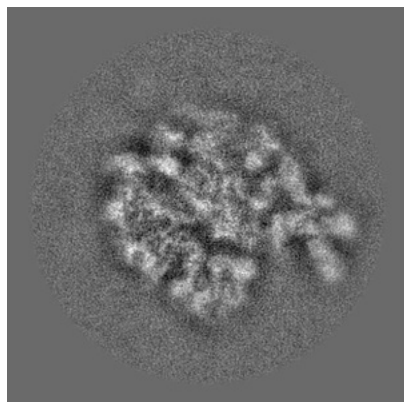


Y Index: 144

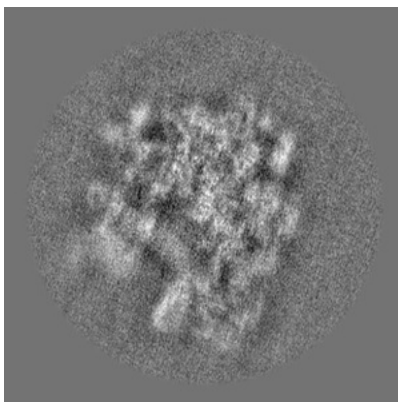


Z Index: 144

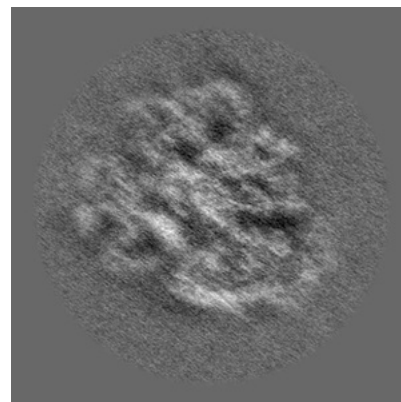
### 6.2.2 Raw map



X Index: 144



Y Index: 144

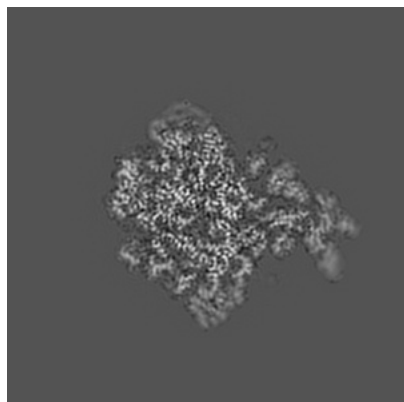


Z Index: 144

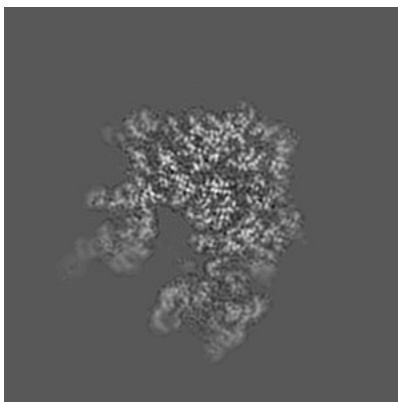
The images above show central slices of the map in three orthogonal directions.

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

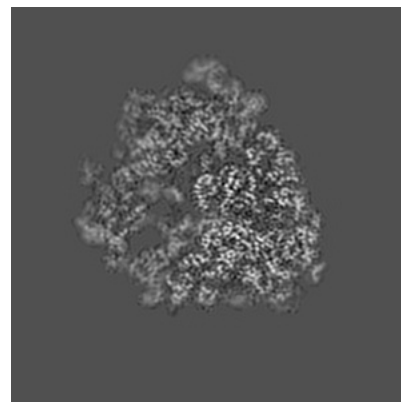
### 6.3.1 Primary map



X Index: 149

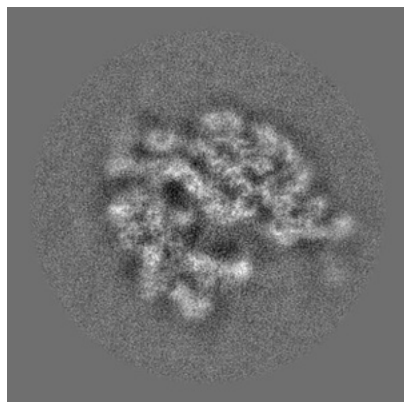


Y Index: 148

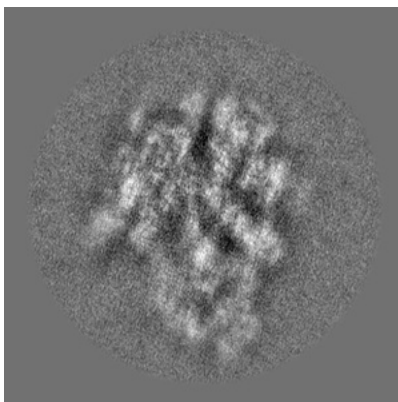


Z Index: 135

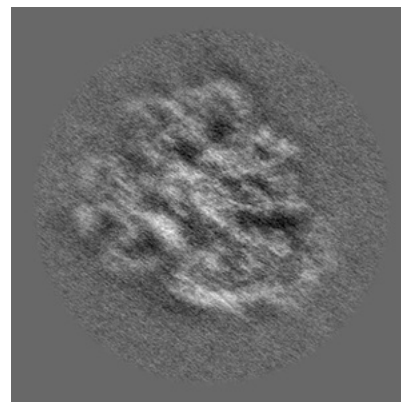
### 6.3.2 Raw map



X Index: 134



Y Index: 129

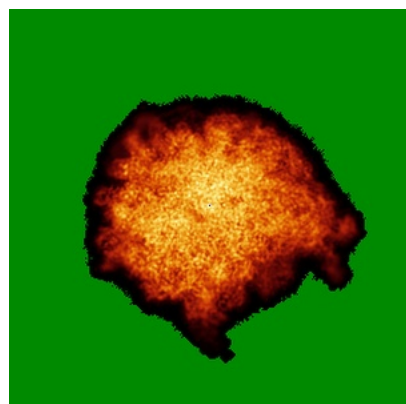


Z Index: 144

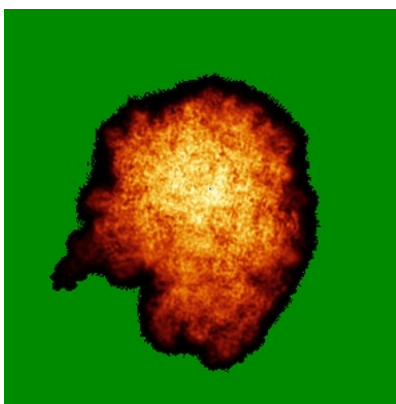
The images above show the largest variance slices of the map in three orthogonal directions.

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

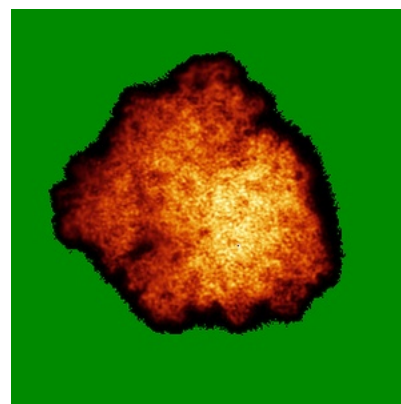
### 6.4.1 Primary map



X

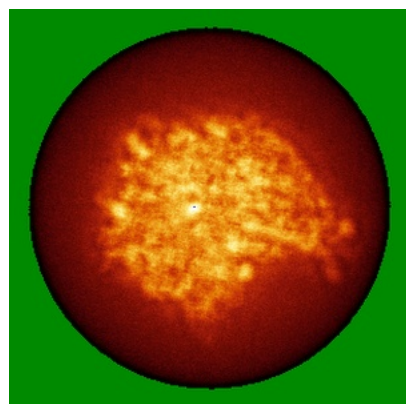


Y

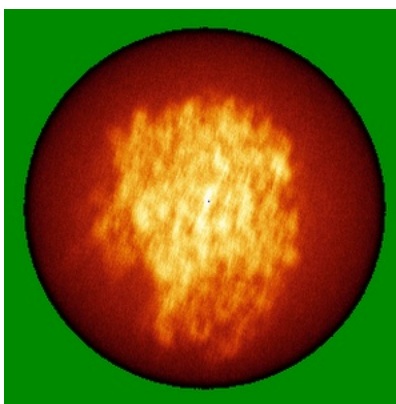


Z

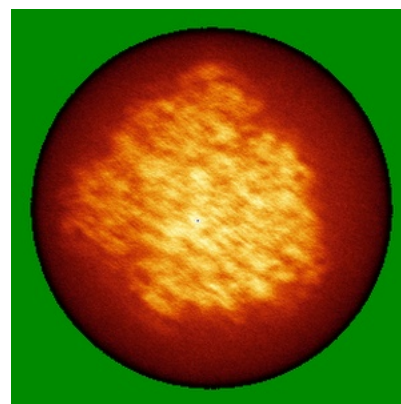
### 6.4.2 Raw map



X



Y



Z

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

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

### 6.5.1 Primary map



X



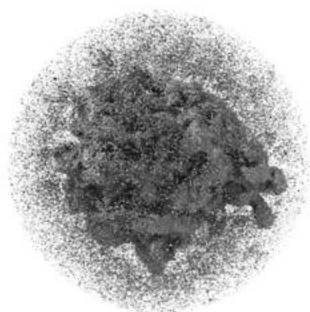
Y



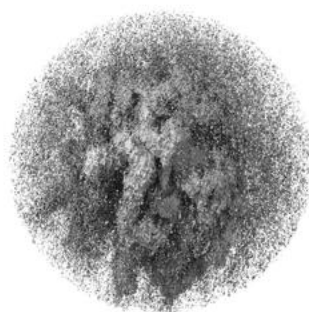
Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

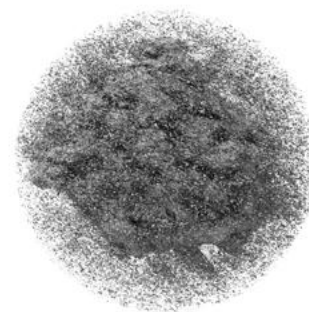
### 6.5.2 Raw map



X



Y



Z

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

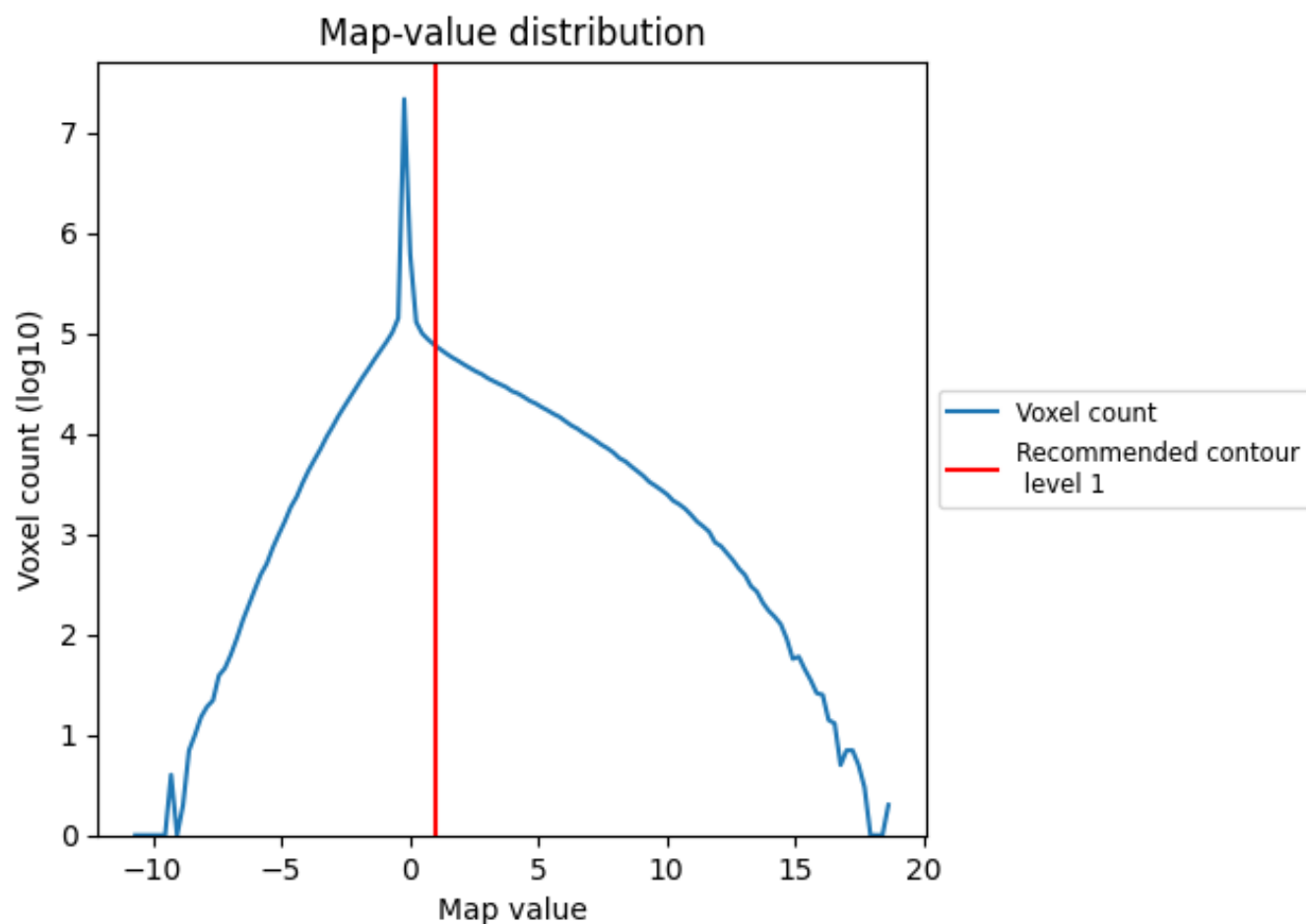
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

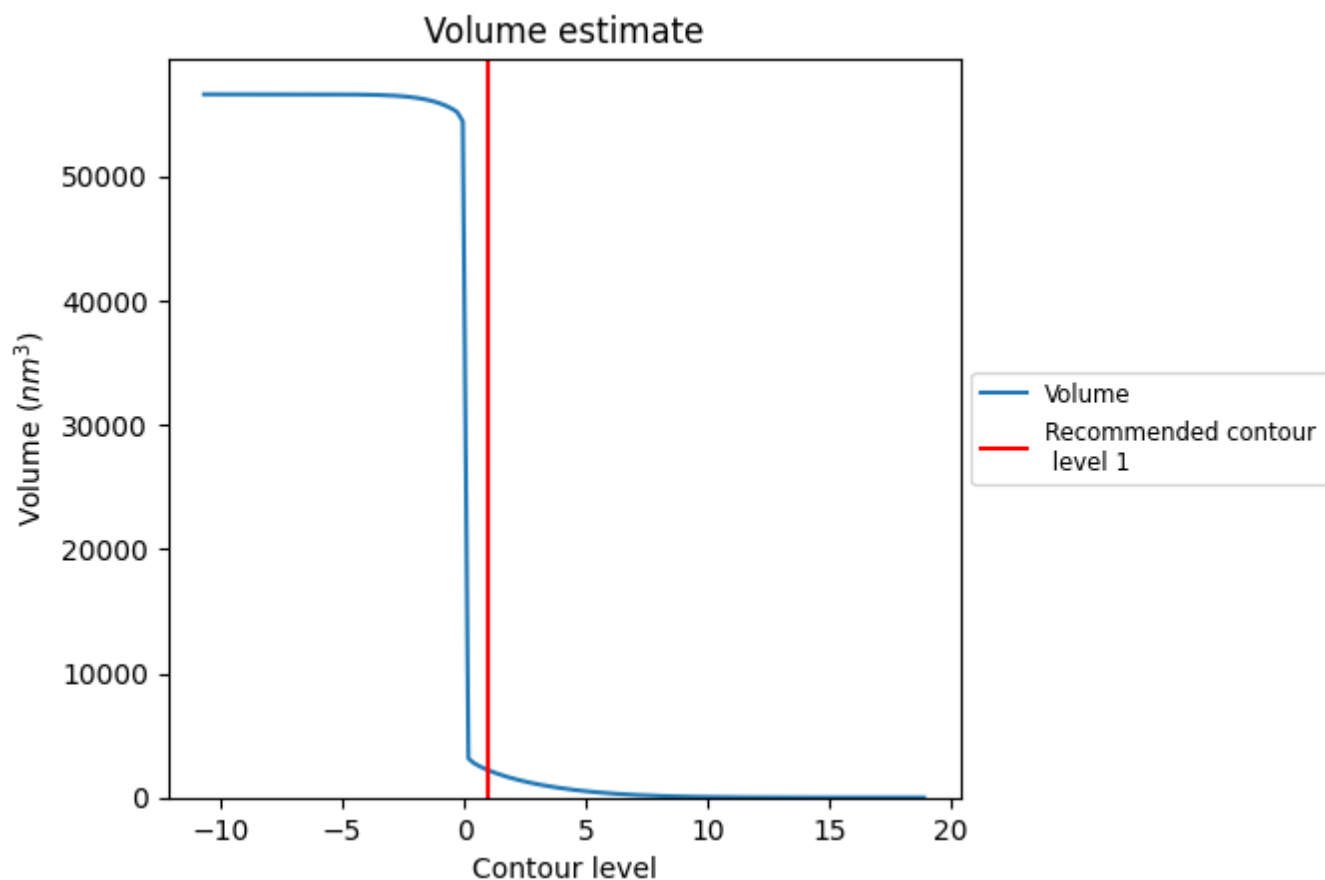
This section contains the results of statistical analysis of the map.

### 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.

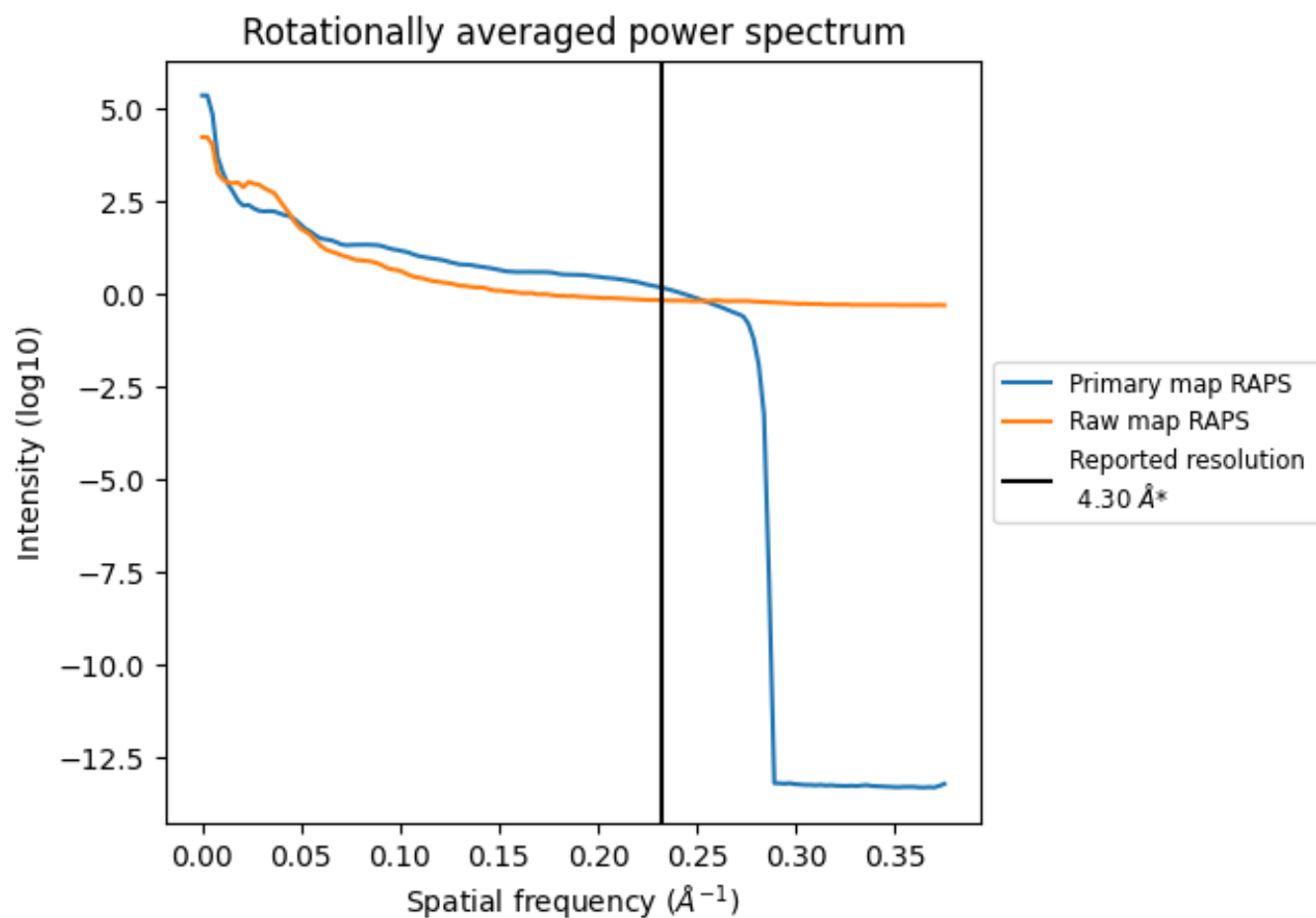
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2191 nm<sup>3</sup>; this corresponds to an approximate mass of 1979 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 ⓘ

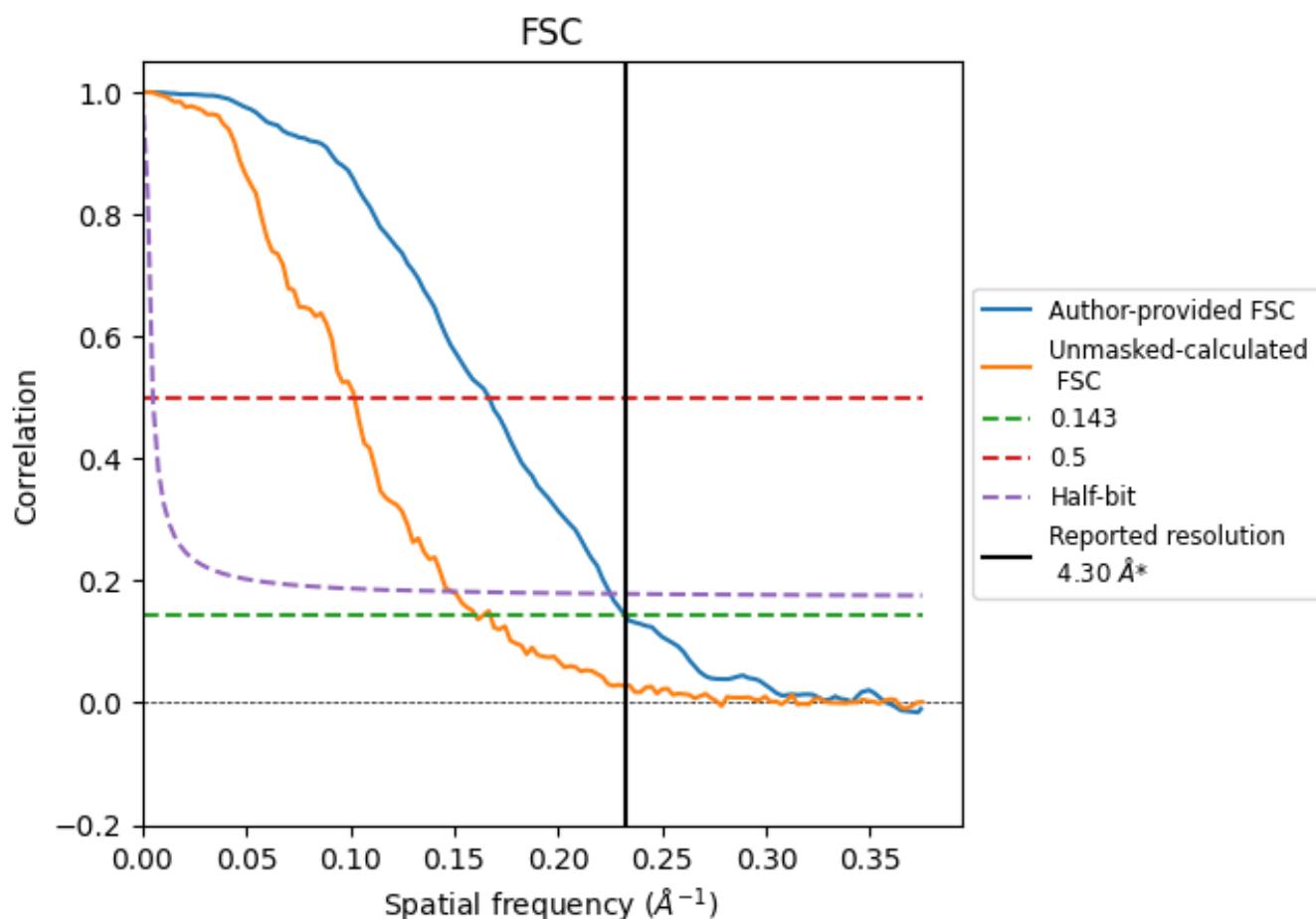


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.233  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

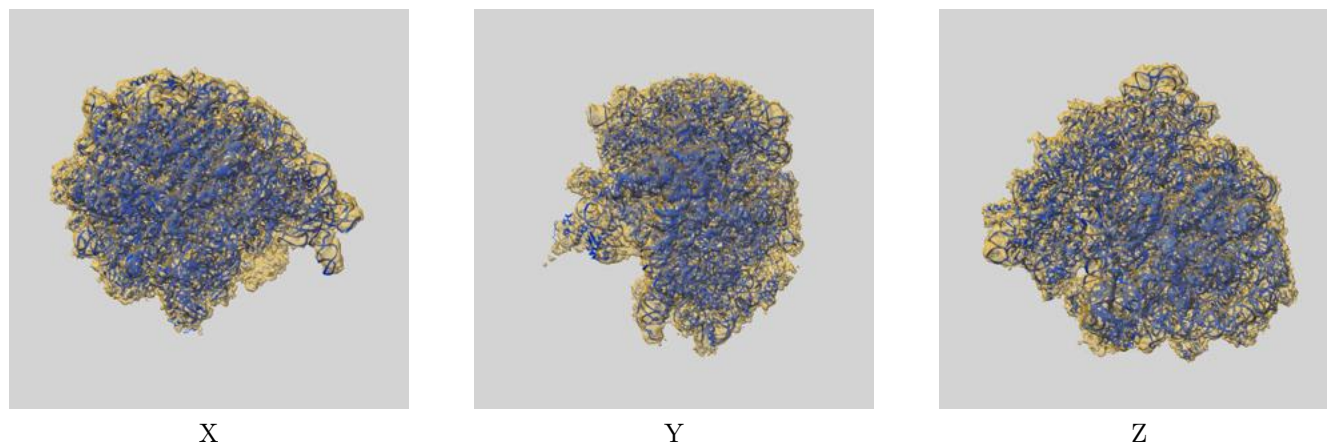
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.30                               | -    | -        |
| Author-provided FSC curve | 4.31                               | 6.00 | 4.44     |
| Unmasked-calculated*      | 6.24                               | 9.80 | 6.71     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.24 differs from the reported value 4.3 by more than 10 %

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

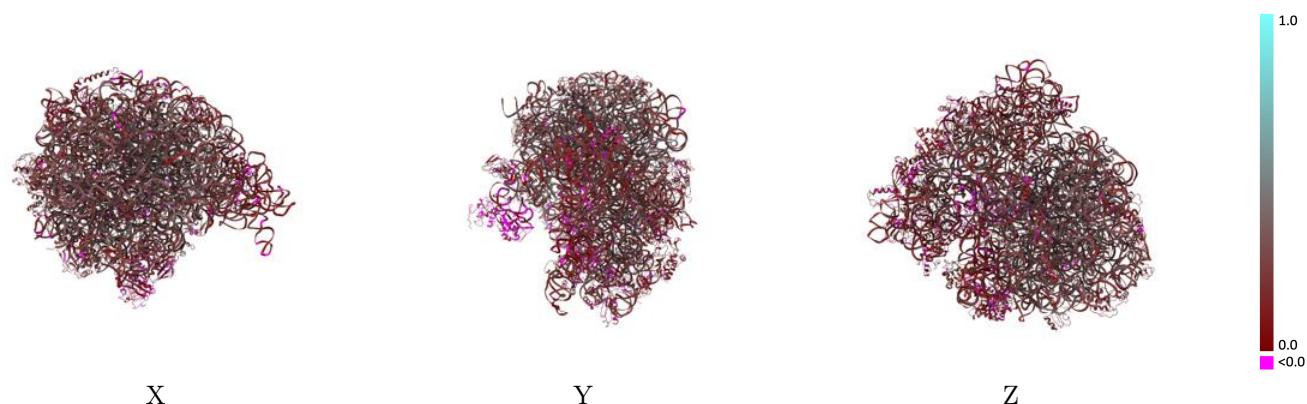
This section contains information regarding the fit between EMDB map EMD-21636 and PDB model 6WDH. Per-residue inclusion information can be found in section 3 on page 15.

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



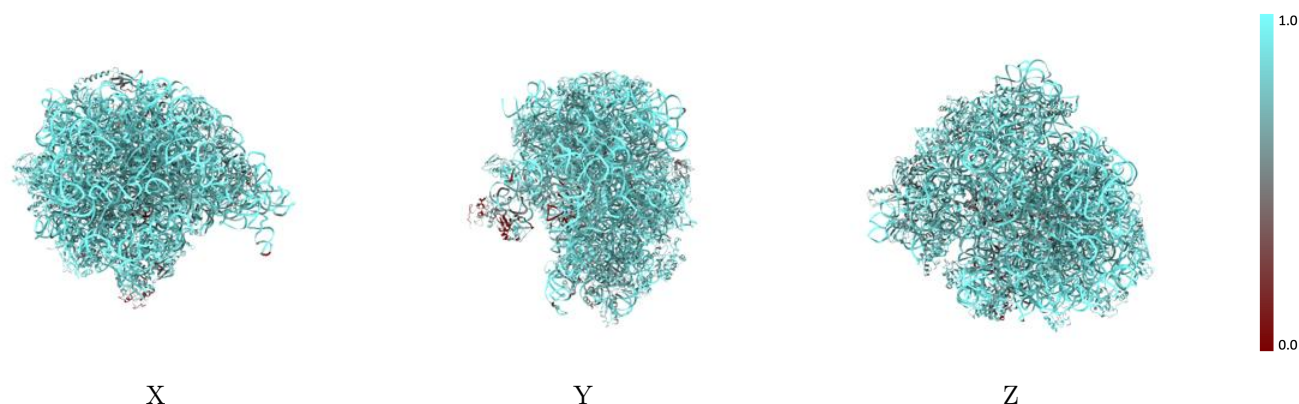
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



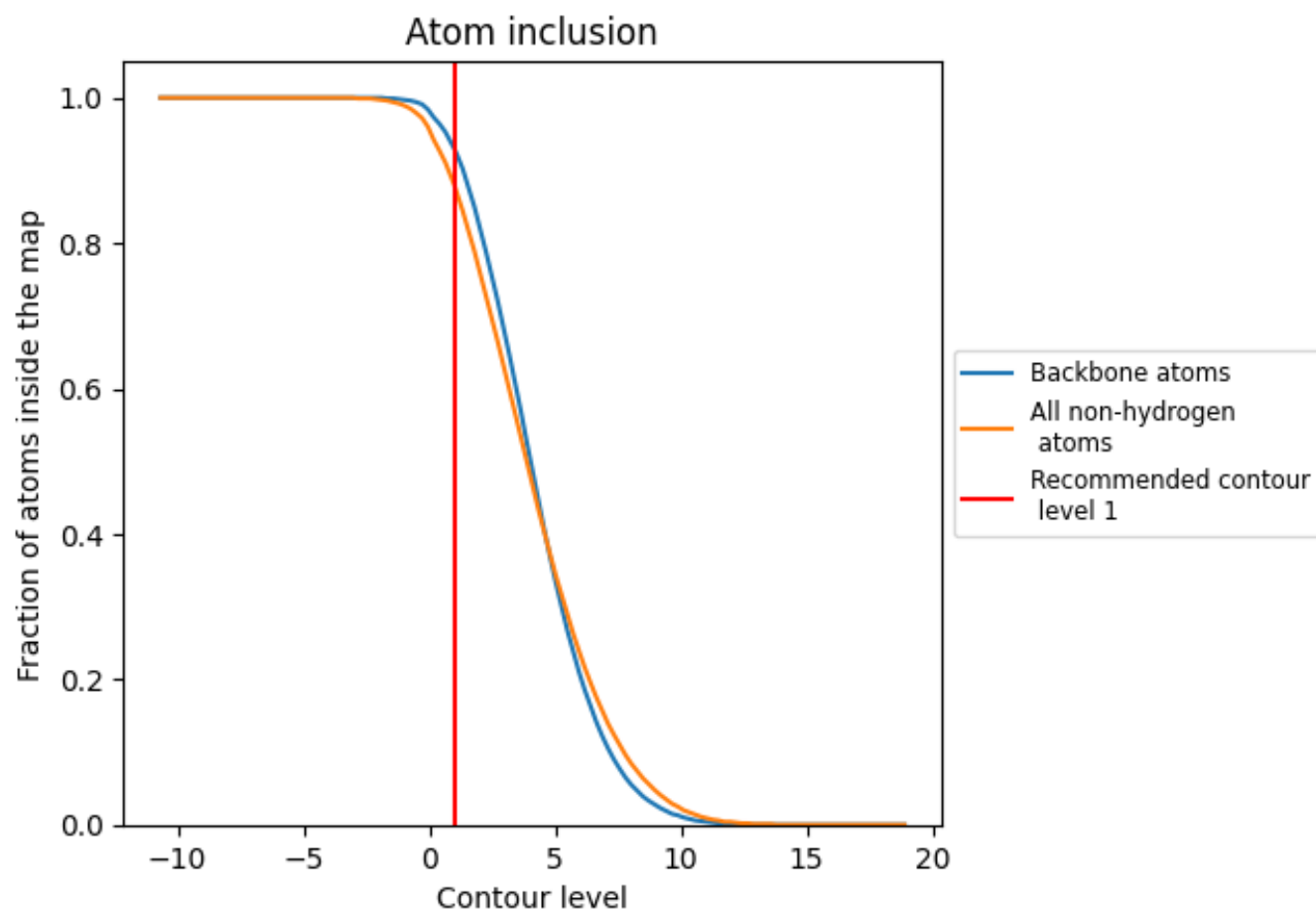
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8790   |  0.2500   |
| 1     |  0.9430   |  0.2970   |
| 2     |  0.9620   |  0.2790   |
| 3     |  0.9230   |  0.2450   |
| 4     |  0.7370   |  0.1340   |
| 5     |  0.8580   |  0.1950   |
| 6     |  0.7560   |  0.1010   |
| 7     |  0.1770   |  0.0080   |
| B     |  0.8460   |  0.2570   |
| C     |  0.6770   |  0.2030   |
| D     |  0.8000   |  0.2850   |
| E     |  0.8450   |  0.3030   |
| F     |  0.7430   |  0.2230   |
| G     |  0.7950   |  0.1920   |
| H     |  0.6960  |  0.1960  |
| I     |  0.7300 |  0.1220 |
| J     |  0.8340 |  0.2760 |
| K     |  0.8470 |  0.1870 |
| L     |  0.8120 |  0.1590 |
| M     |  0.8150 |  0.2300 |
| N     |  0.7750 |  0.1600 |
| O     |  0.6780 |  0.1550 |
| P     |  0.8320 |  0.1910 |
| Q     |  0.7410 |  0.1990 |
| R     |  0.8090 |  0.1480 |
| S     |  0.6670 |  0.1790 |
| T     |  0.8460 |  0.2090 |
| U     |  0.7560 |  0.1670 |
| V     |  0.8170 |  0.1900 |
| W     |  0.8160 |  0.2180 |
| X     |  0.8600 |  0.1910 |
| Y     |  0.7060 |  0.1320 |
| Z     |  0.7570 |  0.1430 |
| a     |  0.6820 |  0.0790 |
| b     |  0.8460 |  0.2820 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| c     |  0.8450   |  0.2790   |
| d     |  0.8390   |  0.2430   |
| e     |  0.8570   |  0.2100   |
| f     |  0.8270   |  0.1690   |
| g     |  0.6900   |  0.1550   |
| h     |  0.4560   |  0.0080   |
| i     |  0.4510   |  -0.0090  |
| j     |  0.8150   |  0.2350   |
| k     |  0.7880   |  0.2560   |
| l     |  0.8400   |  0.2800   |
| m     |  0.8000   |  0.2460   |
| n     |  0.8470   |  0.2850   |
| o     |  0.8520   |  0.2370   |
| p     |  0.8040   |  0.2350   |
| q     |  0.8450   |  0.2820   |
| r     |  0.8360   |  0.2300   |
| s     |  0.8330   |  0.2720   |
| t     |  0.8310  |  0.2550  |
| u     |  0.8310 |  0.2450 |
| v     |  0.8440 |  0.2440 |
| w     |  0.8180 |  0.2750 |
| x     |  0.8600 |  0.2790 |
| y     |  0.7950 |  0.1930 |
| z     |  0.8600 |  0.2590 |