



## Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:48 PM UTC

PDB ID : 6WDK / pdb\_00006wdk  
EMDB ID : EMD-21639  
Title : Cryo-EM of elongating ribosome with EF-Tu\*GTP elucidates tRNA proof-reading (Non-cognate Structure V-A2)  
Authors : Loveland, A.B.; Demo, G.; Korostelev, A.A.  
Deposited on : 2020-03-31  
Resolution : 3.60 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 : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

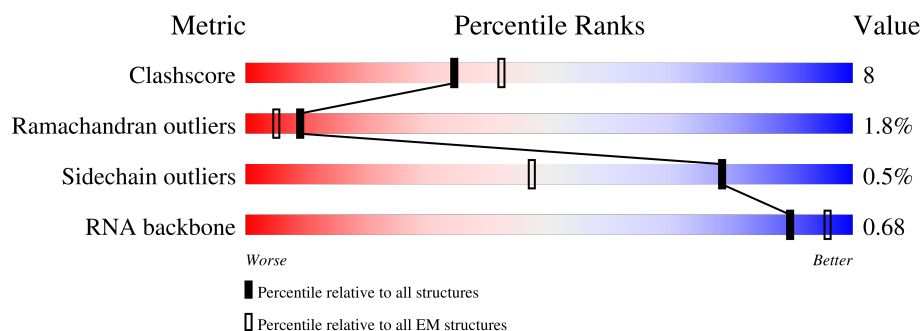
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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.



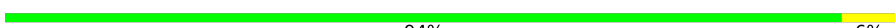
| Metric                | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore            | 229148                   | 23984                    |
| Ramachandran outliers | 224038                   | 23583                    |
| Sidechain outliers    | 223484                   | 23102                    |
| RNA backbone          | 8273                     | 3508                     |

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  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | b     | 271    |                  |
| 2   | c     | 209    |                  |
| 3   | d     | 201    |                  |
| 4   | e     | 177    |                  |
| 5   | f     | 176    |                  |
| 6   | g     | 149    |                  |
| 7   | h     | 131    |                  |

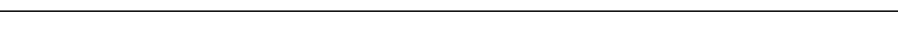
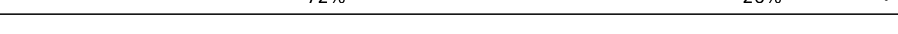
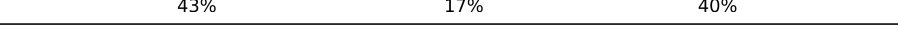
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| Mol | Chain | Length | Quality of chain                                                                                |
|-----|-------|--------|-------------------------------------------------------------------------------------------------|
| 8   | i     | 141    |  71% 28% .    |
| 9   | j     | 142    |  77% 22% .    |
| 10  | k     | 122    |  69% 27% .    |
| 11  | l     | 143    |  78% 20% .    |
| 12  | m     | 136    |  71% 28% .    |
| 13  | n     | 120    |  67% 33%      |
| 14  | o     | 116    |  78% 18% .    |
| 15  | p     | 114    |  68% 29% .    |
| 16  | q     | 117    |  79% 21%      |
| 17  | r     | 103    |  75% 20% 5%   |
| 18  | s     | 110    |  66% 33% .    |
| 19  | t     | 93     |  78% 20% .   |
| 20  | u     | 102    |  71% 28% .  |
| 21  | v     | 94     |  72% 28%    |
| 22  | w     | 75     |  87% 13%    |
| 23  | x     | 77     |  84% 16%    |
| 24  | y     | 63     |  73% 25% .  |
| 25  | z     | 58     |  76% 24%    |
| 26  | B     | 56     |  73% 27%    |
| 27  | C     | 50     |  94% 6%     |
| 28  | D     | 46     |  72% 28%    |
| 29  | E     | 64     |  78% 20% .  |
| 30  | F     | 38     |  61% 34% 5% |
| 31  | G     | 225    |  80% 20%    |
| 32  | H     | 206    |  73% 27%    |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 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   |  |
| 54  | 2     | 120    |  |
| 55  | 5     | 77     |  |
| 55  | 6     | 77     |  |
| 56  | 4     | 18     |  |

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| Mol | Chain | Length | Quality of chain                                                |
|-----|-------|--------|-----------------------------------------------------------------|
| 57  | 7     | 76     | <div><div></div><div>74%</div><div>20%</div><div>7%</div></div> |

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 150222 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       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

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

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

- 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       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- 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       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- 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       | 0     |
|     |       |          | 739   | 466 | 139 | 132 | 2 |         |       |

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

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

- 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 |         |       |

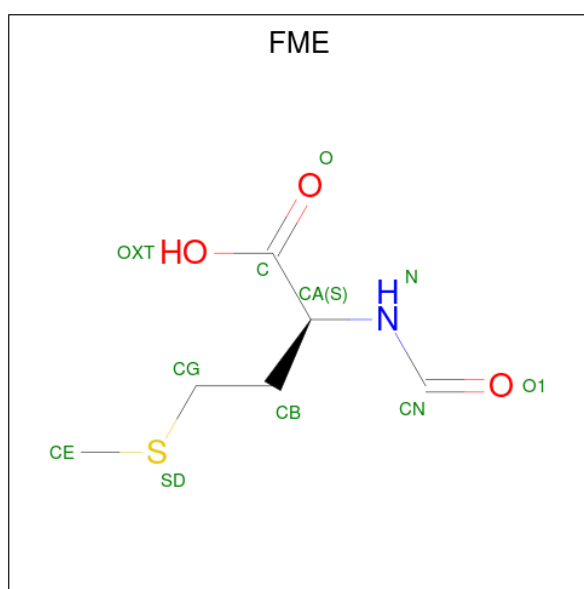
- Molecule 56 is a RNA chain called mRNA.

| 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>P</sup>he.

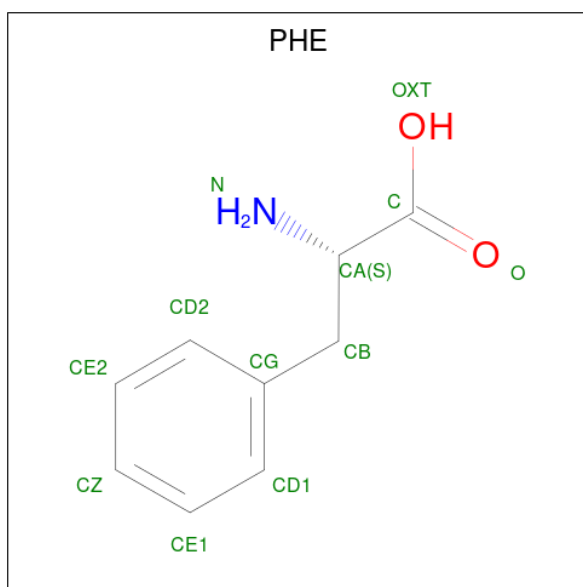
| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 57  | 7     | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1619  | 723 | 290 | 531 | 75 |         |       |

- 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 |         |

- Molecule 59 is PHENYLALANINE (CCD ID: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).

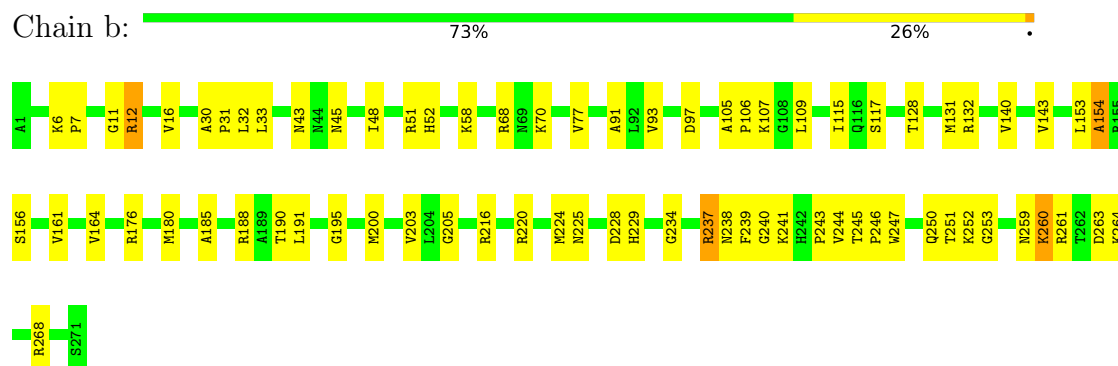


| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
|     |       |          | Total | C | N | O |         |
| 59  | 7     | 1        | 11    | 9 | 1 | 1 | 0       |

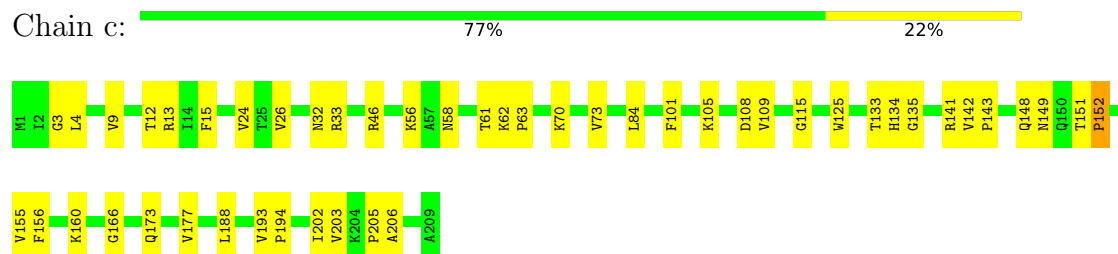
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

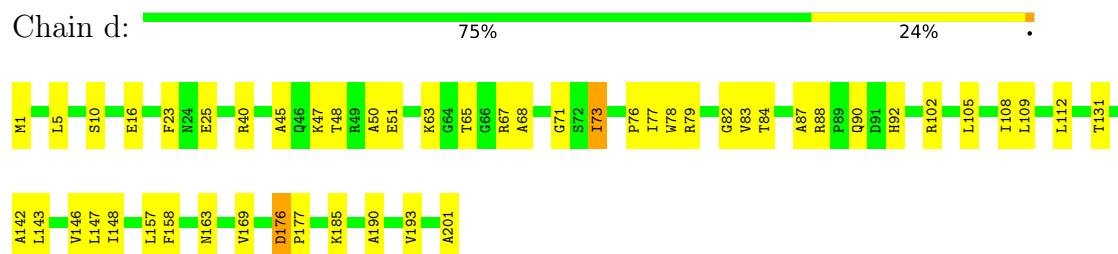
- Molecule 1: 50S ribosomal protein L2



- Molecule 2: 50S ribosomal protein L3

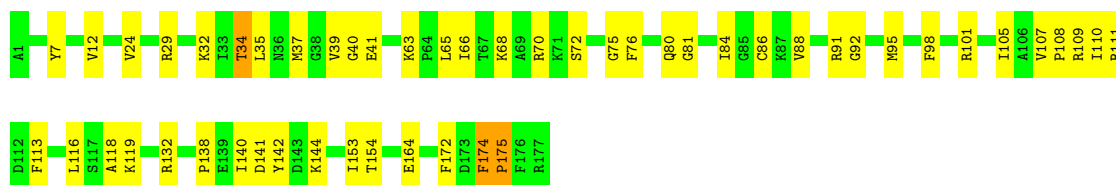


- Molecule 3: 50S ribosomal protein L4



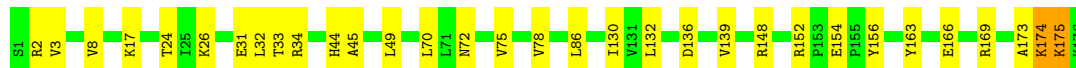
- Molecule 4: 50S ribosomal protein L5





- Molecule 5: 50S ribosomal protein L6

Chain f: 82% 17% .



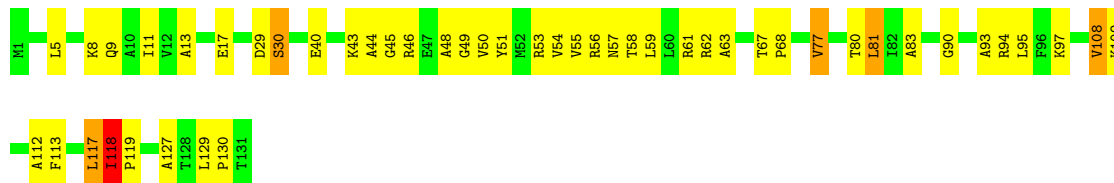
- Molecule 6: 50S ribosomal protein L9

Chain g: 70% 30%



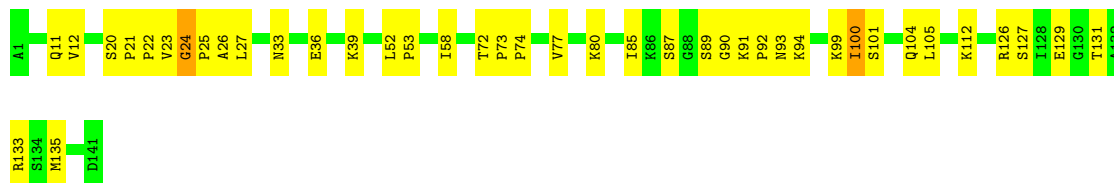
- Molecule 7: 50S ribosomal protein L10

Chain h: 63% 32% . .



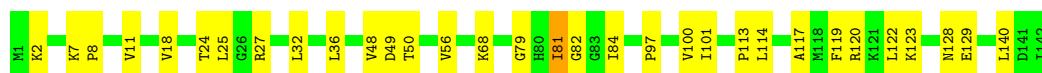
- Molecule 8: 50S ribosomal protein L11

Chain i: 71% 28% .

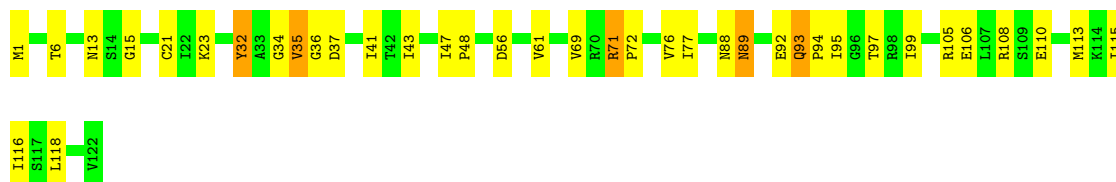


- Molecule 9: 50S ribosomal protein L13

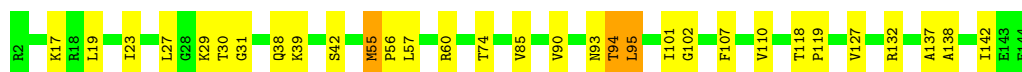
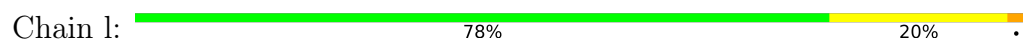
Chain j: 77% 22% .



- Molecule 10: 50S ribosomal protein L14



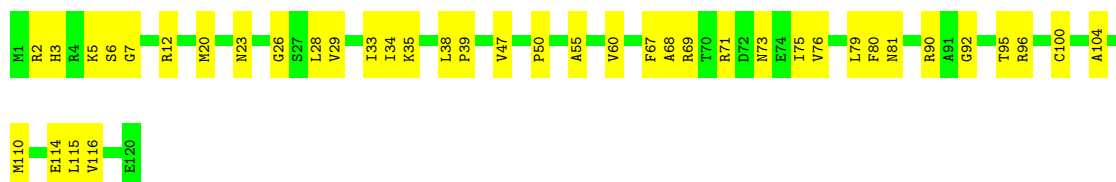
- Molecule 11: 50S ribosomal protein L15



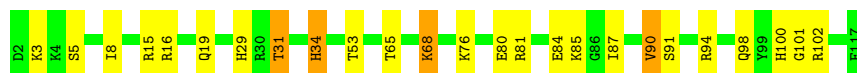
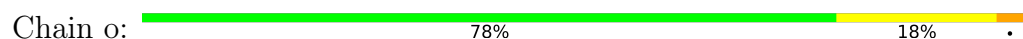
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17

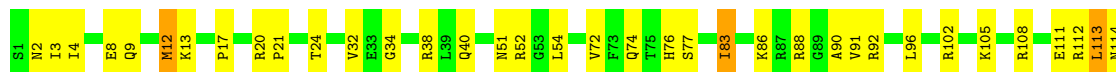


- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19

Chain p:  68% 29% .



- Molecule 16: 50S ribosomal protein L20

Chain q:  79% 21%



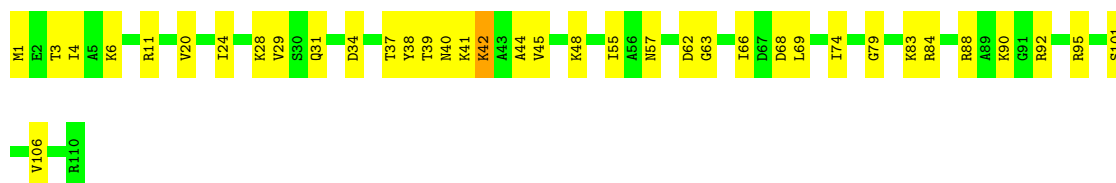
- Molecule 17: 50S ribosomal protein L21

Chain r:  75% 20% 5%



- Molecule 18: 50S ribosomal protein L22

Chain s:  66% 33%



- Molecule 19: 50S ribosomal protein L23

Chain t:  78% 20%



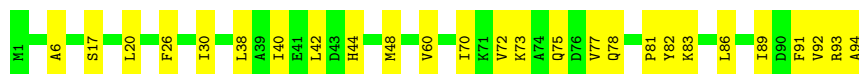
- Molecule 20: 50S ribosomal protein L24

Chain u:  71% 28%



- Molecule 21: 50S ribosomal protein L25

Chain v:  72% 28%



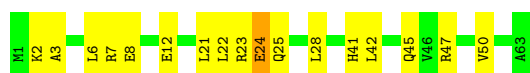
## • Molecule 22: 50S ribosomal protein L27

Chain w:  87% 13%

## • Molecule 23: 50S ribosomal protein L28

Chain x:  84% 16%

## • Molecule 24: 50S ribosomal protein L29

Chain y:  73% 25% .

## • Molecule 25: 50S ribosomal protein L30

Chain z:  76% 24%

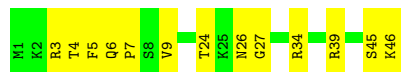
## • Molecule 26: 50S ribosomal protein L32

Chain B:  73% 27%

## • Molecule 27: 50S ribosomal protein L33

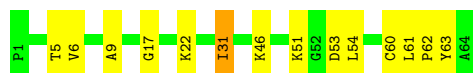
Chain C:  94% 6%

## • Molecule 28: 50S ribosomal protein L34

Chain D:  72% 28%

## • Molecule 29: 50S ribosomal protein L35

Chain E:  78% 20% .



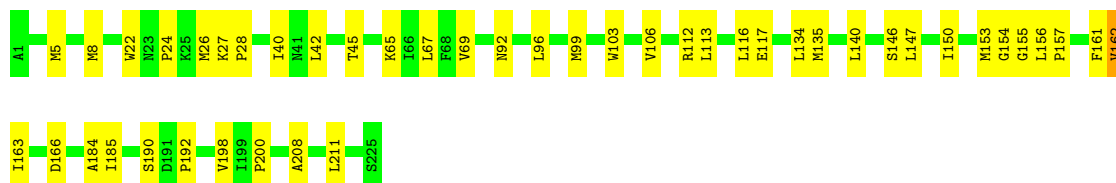
- Molecule 30: 50S ribosomal protein L36

Chain F:  61% 34% 5%



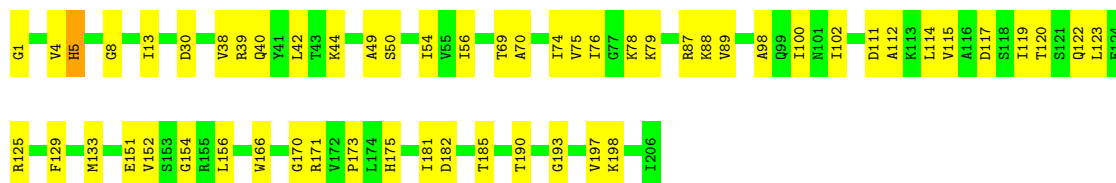
- Molecule 31: 30S ribosomal protein S2

Chain G:  80% 20%



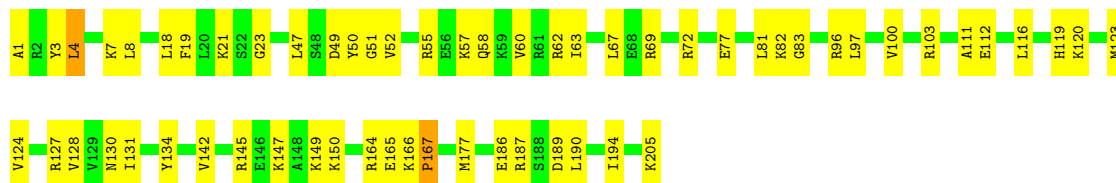
- Molecule 32: 30S ribosomal protein S3

Chain H:  73% 27%



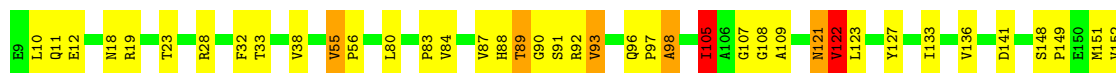
- Molecule 33: 30S ribosomal protein S4

Chain I:  71% 28% .



- Molecule 34: 30S ribosomal protein S5

Chain J:  73% 22% . .





- Molecule 35: 30S ribosomal protein S6

Chain K: 62% 32% 6%



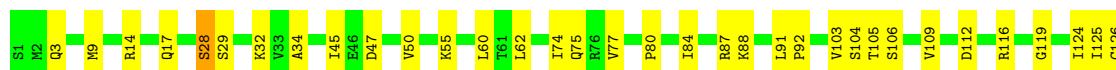
- Molecule 36: 30S ribosomal protein S7

Chain L: 63% 34% .



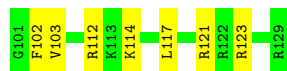
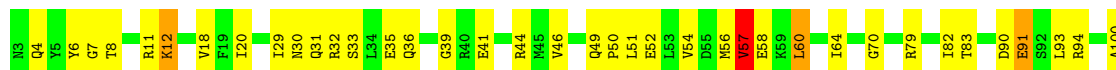
- Molecule 37: 30S ribosomal protein S8

Chain M: 74% 26% .



- Molecule 38: 30S ribosomal protein S9

Chain N: 65% 32% ..

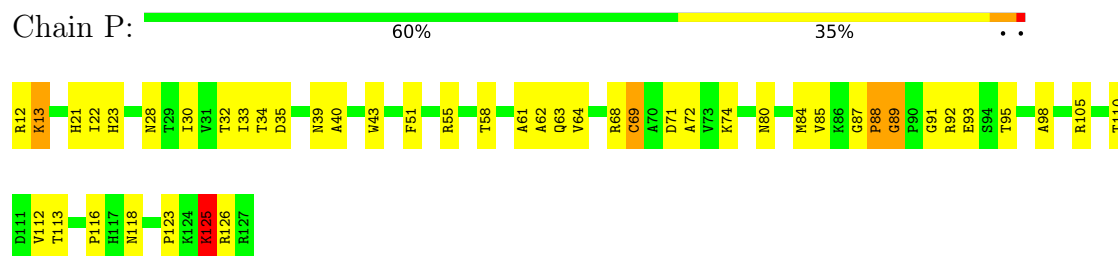


- Molecule 39: 30S ribosomal protein S10

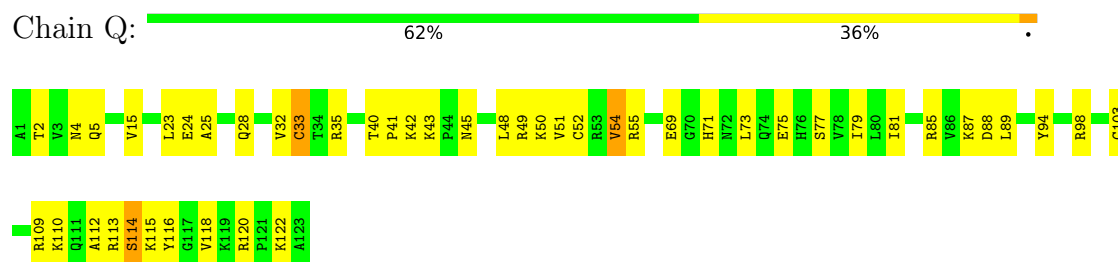
Chain O: 67% 30% ..



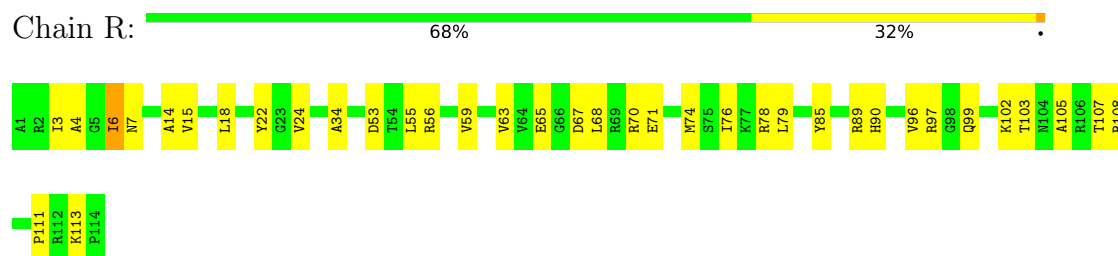
- Molecule 40: 30S ribosomal protein S11



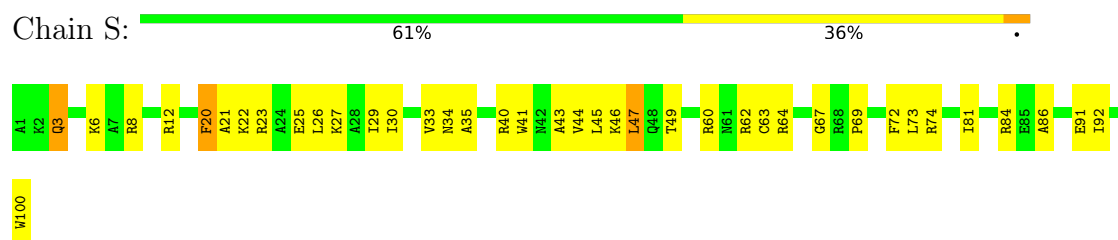
- Molecule 41: 30S ribosomal protein S12



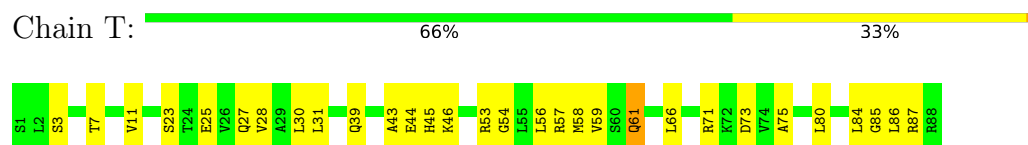
- Molecule 42: 30S ribosomal protein S13



- Molecule 43: 30S ribosomal protein S14



- Molecule 44: 30S ribosomal protein S15



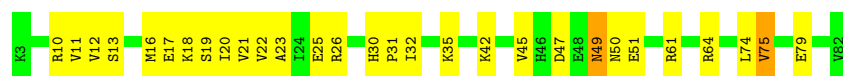
- Molecule 45: 30S ribosomal protein S16

Chain U:  66% 29% 5%



- Molecule 46: 30S ribosomal protein S17

Chain V:  64% 34% .



- Molecule 47: 30S ribosomal protein S18

Chain W:  72% 26% .



- Molecule 48: 30S ribosomal protein S19

Chain X:  66% 34%



- Molecule 49: 30S ribosomal protein S20

Chain Y:  71% 29%

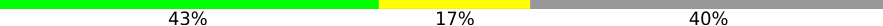


- Molecule 50: 30S ribosomal protein S21

Chain Z:  57% 37% 6%



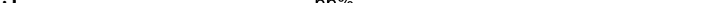
- Molecule 51: 50S ribosomal protein L1

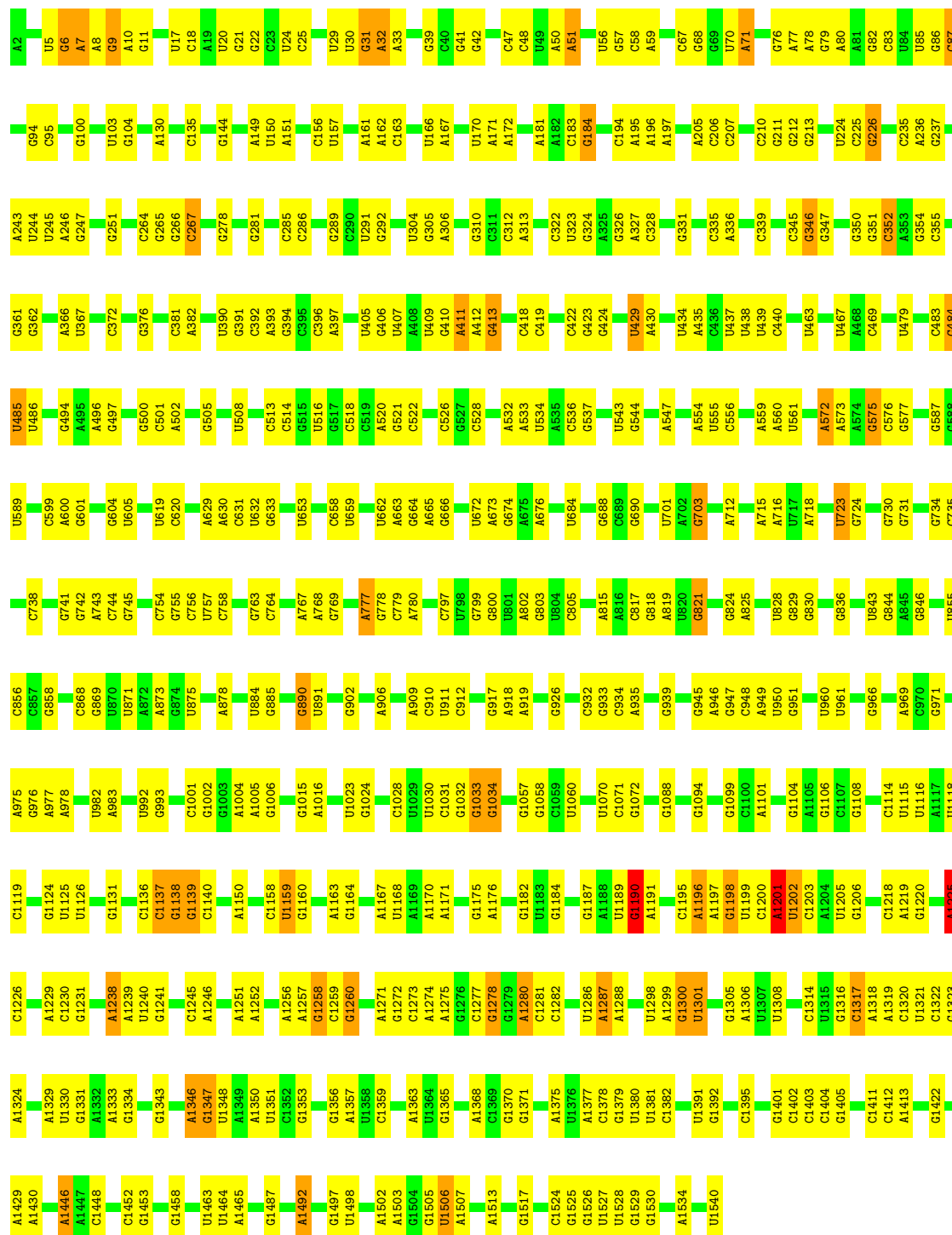
Chain a:  43% 17% 40%



ALA GLU LEU VAL GLY MET GLU ASP LEU ALA ASP GLN ILE LYS LYS GLY A28 GLU L29 MET ASN PHE ASP VAL ILE ALA SER PRO ASP ALA MET ARG VAL Y59 GLY G61 GLN LEU GLY GLN T69 GLY VAL LEU ARG GLY PRO ARG LEU MET PHE PRO ASN THR VAL THR ALA ASN VAL ALA GLU THR PRO ASN VAL ALA GLU

- Molecule 52: 16S ribosomal RNA

Chain 3:  66% 31% 3%

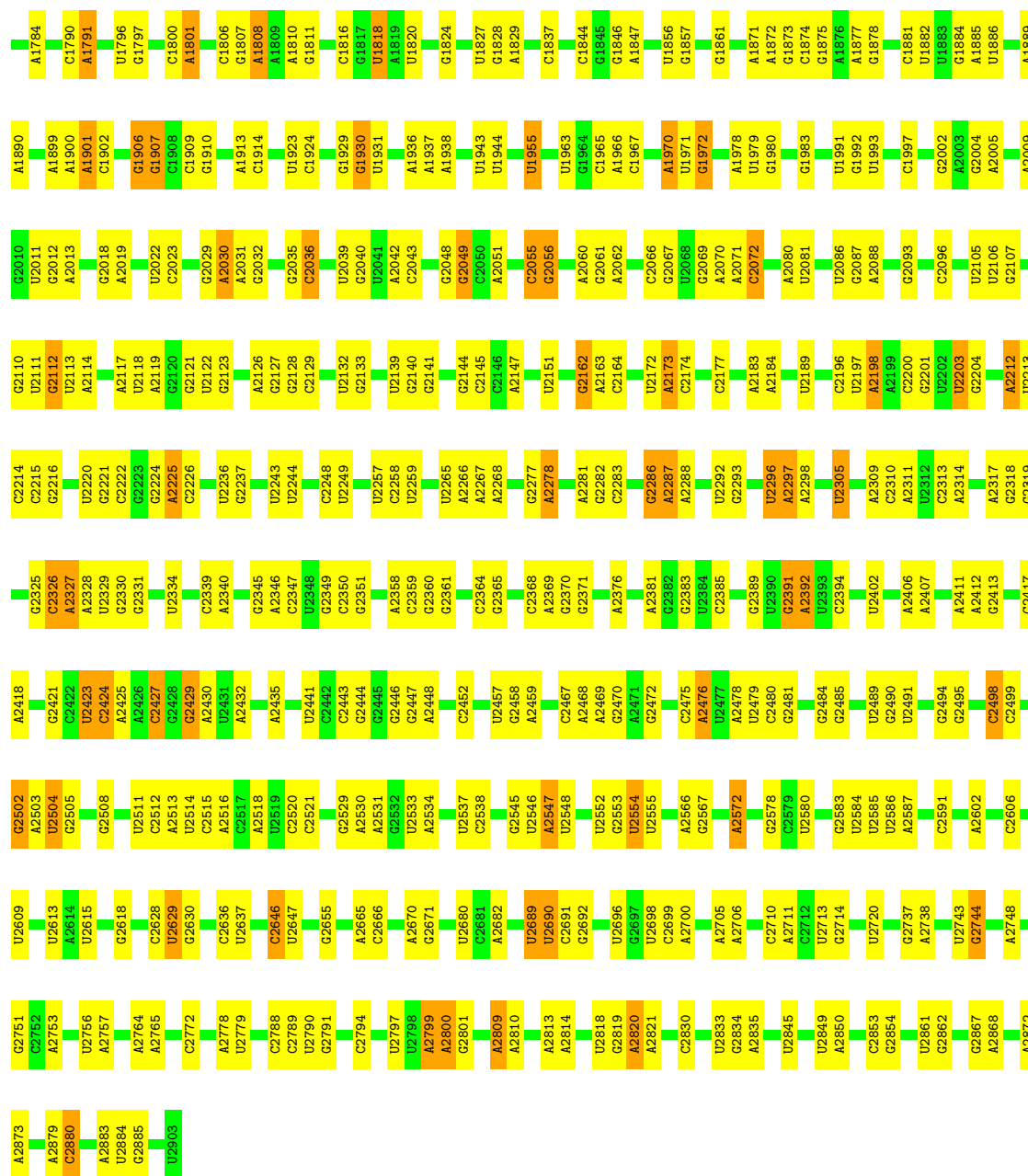


- Molecule 53: 23S ribosomal RNA

Chain 1:

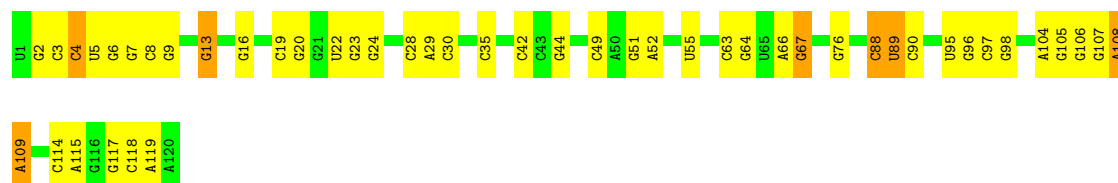


|      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |
|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|
| G1   | C129 | C240 | U360 | G458 | U558 | G669 | A781 | C865 | G997  | U1097 | G1212 | U1344 | A1490 | G1616 |
| G7   | C130 | A241 | G361 | A458 | G559 | A670 | A782 | U871 | A1010 | A1103 | U1231 | C1345 | G1491 | A1636 |
| A10  | U135 | U243 | G363 | A466 | C560 | C672 | G784 | U872 | G1011 | C1104 | U1232 | A1354 | A1494 | A1637 |
| C11  | G136 | A244 | G367 | A470 | G561 | C673 | G785 | G674 | U1012 | U1105 | C873  | G1355 | A1495 | G1645 |
| U12  | U137 | G248 | A368 | A473 | A563 | A675 | A792 | G875 | A1014 | G1107 | G1250 | G1356 | A1496 | G1646 |
| A13  | U138 | C249 | U369 | G474 | U566 | A676 | A793 | C876 | U1015 | G1110 | G1251 | G1357 | A1497 | U1648 |
| G17  | C140 | A142 | G370 | G474 | A572 | C682 | C795 | A878 | U1016 | A1111 | G1252 | A1359 | C1498 |       |
| A28  | G141 | C253 | A371 | A477 | U573 | U686 | G796 | C885 | A1020 | G1112 | A1253 | A1254 | C1507 | G1651 |
| U34  | A149 | A255 | U373 | A478 | U577 | C687 | G797 | A886 | A1021 | U1113 | U1255 | A1256 | A1508 | G1656 |
| G35  | U150 | A256 | A374 | A479 | G577 | U688 | G798 | U887 | G1022 | G1122 | G1257 | A1367 | A1509 |       |
| C45  | C151 | G285 | G375 | A480 | U578 | U689 | A800 | C888 | U1023 | G1125 | G1258 | G1368 | G1510 |       |
| G46  | A152 | A286 | U387 | A482 | G579 | A690 | G801 | C899 | G1026 | G1125 | U1259 | A1369 | A1515 | G1666 |
| A49  | A161 | C275 | A391 | G488 | U580 | C691 | A802 | A896 | A1027 | G1130 | A1264 | C1370 | G1524 | G1674 |
| U50  | U162 | U276 | A392 | G489 | A582 | U694 | G805 | C897 | A1028 | G1131 | A1268 | U1371 | A1525 | G1683 |
| G51  | C163 | G277 | U395 | C490 | G583 | G695 | G806 | C898 | U1033 | U1132 | A1269 | U1372 | A1526 | G1684 |
| C57  | A165 | A278 | G396 | C491 | G585 | U703 | G808 | A905 | G1034 | A1133 | G1270 | A1373 | G1527 |       |
| G58  | U171 | U280 | A401 | A492 | G588 | G704 | G809 | U906 | U1035 | A1134 | C1271 | C1376 | A1528 | G1687 |
| A63  | A172 | C281 | A404 | C494 | U588 | A706 | U810 | A910 | G1036 | C1135 | A1272 | G1377 | G1529 |       |
| C69  | A176 | U290 | A405 | G498 | U596 | G707 | C812 | G923 | G1042 | G1138 | A1275 | U1378 | A1535 | G1689 |
| G70  | G177 | G291 | G406 | U499 | G597 | G713 | C815 | G924 | C1043 | G1139 | A1276 | U1379 | C1536 |       |
| A71  | A181 | A294 | G407 | A503 | U598 | A718 | C816 | A943 | G1044 | C1140 | C1278 | A1383 | G1537 | U1709 |
| A74  | G189 | G301 | G411 | A505 | A603 | C723 | C817 | G946 | A1045 | U1141 | G1279 | A1384 | G1538 | G1710 |
| G75  | A190 | C305 | C414 | C506 | U610 | U724 | A819 | A941 | A1046 | A1142 | U1285 | U1394 | U1539 | G1715 |
| U78  | C192 | U306 | U416 | G512 | C611 | G725 | A820 | A943 | A1047 | A1143 | A1286 | A1395 | C1560 |       |
| A84  | A196 | G307 | C421 | C523 | U615 | A727 | U826 | C946 | U1060 | G1153 | C1297 | U1415 | G1565 | U1720 |
| G85  | G205 | A310 | A422 | G524 | G617 | G728 | U827 | G954 | U1061 | G1154 | G1298 | G1416 | A1566 | G1721 |
| A91  | C213 | A311 | A423 | A528 | A627 | A730 | U828 | A959 | G1062 | G1157 | A1301 | G1417 | A1569 |       |
| U92  | G214 | G312 | G424 | A529 | A631 | G738 | C830 | C961 | U1066 | C1161 | C1306 | A1419 | A1570 | G1736 |
| C96  | G215 | A319 | C433 | C531 | A632 | A739 | A833 | G967 | A1070 | G1162 | G1309 | G1432 | A1571 | G1737 |
| G97  | A216 | A320 | U434 | A532 | A637 | U741 | G834 | C968 | A1071 | A1175 | C1310 | A1433 | G1581 | G1738 |
| G98  | A219 | U321 | C435 | G533 | A639 | A742 | G835 | G969 | C1076 | U1176 | C1319 | G1437 | U1584 | G1739 |
| U102 | G220 | A322 | U437 | G535 | U639 | A743 | U839 | U970 | A1077 | G1177 | C1320 | U1438 | A1587 | G1740 |
| U112 | A221 | A323 | A439 | G538 | C640 | C747 | A845 | G971 | U1078 | G1178 | U1326 | A1439 | A1603 |       |
| U113 | A222 | G327 | A440 | A538 | A644 | A752 | U846 | G973 | A1080 | U1180 | A1327 | C1454 | C1606 | G1758 |
| A118 | U224 | U328 | U441 | G539 | A645 | U755 | C854 | G974 | U1083 | U1183 | A1328 | C1455 | C1607 | C1764 |
| A119 | C225 | A330 | A442 | C542 | U646 | A756 | G855 | A975 | A1084 | G1186 | U1329 | C1456 | A1608 | A1772 |
| U120 | A226 | A340 | A443 | G543 | U651 | U763 | G859 | A983 | A1088 | G1187 | C1330 | G1461 | A1609 | A1773 |
| C121 | A227 | C341 | U448 | U545 | A654 | A764 | U860 | C987 | A1093 | U1189 | G1332 | U1474 | A1610 | G1774 |
| G122 | G230 | A342 | U451 | A547 | A654 | A766 | A861 | A988 | G1094 | U1190 | G1333 | G1475 | C1611 | G1775 |
| G123 | A231 | A346 | C455 | U554 | G664 | G776 | G862 | C995 | U1095 | A1204 | A1336 | U1476 | C1612 | U1779 |
| G124 | C239 | G359 | A457 | G555 | A668 | G780 | G864 | A996 | A1096 | A1205 | G1482 |       | G1613 | A1780 |



• Molecule 54: 5S ribosomal RNA

Chain 2: 60% 34% 6%



• Molecule 55: tRNA<sup>fMet</sup>

Chain 5: 73% 23% 4%



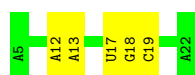
- Molecule 55: tRNAfMet

Chain 6: 73% 23% .



- Molecule 56: mRNA

Chain 4: 72% 28%



- Molecule 57: tRNAPhe

Chain 7: 74% 20% 7%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 11041                                   | 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 |

## 5 Model quality

### 5.1 Standard geometry

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     | 0.28         | 0/2122  | 0.90        | 4/2852 (0.1%) |
| 2   | c     | 0.28         | 0/1586  | 0.83        | 2/2134 (0.1%) |
| 3   | d     | 0.28         | 0/1571  | 0.85        | 4/2113 (0.2%) |
| 4   | e     | 0.30         | 0/1435  | 0.89        | 5/1926 (0.3%) |
| 5   | f     | 0.29         | 0/1343  | 0.85        | 1/1816 (0.1%) |
| 6   | g     | 0.30         | 0/1122  | 0.92        | 0/1515        |
| 7   | h     | 0.34         | 0/1002  | 0.97        | 3/1350 (0.2%) |
| 8   | i     | 0.34         | 0/1046  | 0.94        | 3/1410 (0.2%) |
| 9   | j     | 0.28         | 0/1152  | 0.86        | 2/1551 (0.1%) |
| 10  | k     | 0.27         | 0/948   | 0.93        | 4/1268 (0.3%) |
| 11  | l     | 0.29         | 0/1054  | 0.90        | 4/1403 (0.3%) |
| 12  | m     | 0.28         | 0/1093  | 0.78        | 0/1460        |
| 13  | n     | 0.30         | 0/974   | 0.90        | 3/1301 (0.2%) |
| 14  | o     | 0.28         | 0/902   | 0.86        | 1/1209 (0.1%) |
| 15  | p     | 0.28         | 0/929   | 0.83        | 0/1242        |
| 16  | q     | 0.28         | 0/960   | 0.88        | 2/1278 (0.2%) |
| 17  | r     | 0.29         | 0/829   | 0.79        | 1/1107 (0.1%) |
| 18  | s     | 0.27         | 0/864   | 0.90        | 4/1156 (0.3%) |
| 19  | t     | 0.26         | 0/745   | 0.78        | 1/994 (0.1%)  |
| 20  | u     | 0.27         | 0/788   | 0.87        | 0/1051        |
| 21  | v     | 0.27         | 0/766   | 0.76        | 0/1025        |
| 22  | w     | 0.27         | 0/582   | 0.80        | 0/769         |
| 23  | x     | 0.27         | 0/635   | 0.85        | 2/848 (0.2%)  |
| 24  | y     | 0.27         | 0/510   | 0.91        | 1/677 (0.1%)  |
| 25  | z     | 0.29         | 0/453   | 0.78        | 0/605         |
| 26  | B     | 0.28         | 0/450   | 0.77        | 0/599         |
| 27  | C     | 0.32         | 0/417   | 0.82        | 0/554         |
| 28  | D     | 0.32         | 0/380   | 1.03        | 3/498 (0.6%)  |
| 29  | E     | 0.28         | 0/513   | 0.89        | 1/676 (0.1%)  |
| 30  | F     | 0.30         | 0/303   | 0.89        | 2/397 (0.5%)  |
| 31  | G     | 0.30         | 0/1788  | 0.87        | 3/2408 (0.1%) |
| 32  | H     | 0.30         | 0/1652  | 0.89        | 6/2225 (0.3%) |

| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 33  | I     | 0.29         | 0/1665   | 0.88        | 2/2227 (0.1%)     |
| 34  | J     | 0.31         | 0/1170   | 0.93        | 5/1573 (0.3%)     |
| 35  | K     | 0.31         | 0/836    | 0.95        | 3/1128 (0.3%)     |
| 36  | L     | 0.28         | 0/1196   | 0.94        | 5/1602 (0.3%)     |
| 37  | M     | 0.28         | 0/989    | 0.86        | 3/1326 (0.2%)     |
| 38  | N     | 0.29         | 0/1034   | 0.89        | 3/1375 (0.2%)     |
| 39  | O     | 0.33         | 0/797    | 0.90        | 0/1077            |
| 40  | P     | 0.31         | 0/886    | 0.92        | 3/1195 (0.3%)     |
| 41  | Q     | 0.30         | 0/969    | 0.99        | 3/1300 (0.2%)     |
| 42  | R     | 0.30         | 0/893    | 0.92        | 4/1193 (0.3%)     |
| 43  | S     | 0.29         | 0/817    | 0.88        | 2/1088 (0.2%)     |
| 44  | T     | 0.28         | 0/722    | 0.91        | 4/964 (0.4%)      |
| 45  | U     | 0.31         | 0/659    | 0.91        | 2/884 (0.2%)      |
| 46  | V     | 0.26         | 0/658    | 0.99        | 3/881 (0.3%)      |
| 47  | W     | 0.32         | 0/545    | 1.01        | 4/731 (0.5%)      |
| 48  | X     | 0.32         | 0/653    | 0.90        | 1/877 (0.1%)      |
| 49  | Y     | 0.29         | 0/671    | 0.93        | 4/888 (0.5%)      |
| 50  | Z     | 0.34         | 0/551    | 1.01        | 3/728 (0.4%)      |
| 51  | a     | 0.30         | 0/1034   | 0.79        | 0/1387            |
| 52  | 3     | 0.40         | 0/36963  | 0.50        | 5/57662 (0.0%)    |
| 53  | 1     | 0.39         | 0/69796  | 0.50        | 2/108888 (0.0%)   |
| 54  | 2     | 0.40         | 0/2872   | 0.50        | 0/4479            |
| 55  | 5     | 0.40         | 0/1832   | 0.47        | 0/2855            |
| 55  | 6     | 0.40         | 0/1832   | 0.52        | 0/2855            |
| 56  | 4     | 0.40         | 0/436    | 0.49        | 0/679             |
| 57  | 7     | 0.39         | 0/1809   | 0.48        | 0/2819            |
| All | All   | 0.37         | 0/163199 | 0.62        | 123/244078 (0.1%) |

There are no bond length outliers.

All (123) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 46  | V     | 75  | VAL  | N-CA-C | -11.00 | 102.10      | 111.56   |
| 1   | b     | 259 | ASN  | N-CA-C | -8.62  | 104.79      | 114.62   |
| 50  | Z     | 21  | SER  | N-CA-C | -8.37  | 102.63      | 112.92   |
| 28  | D     | 6   | GLN  | CA-C-N | 8.15   | 128.17      | 119.78   |
| 28  | D     | 6   | GLN  | C-N-CA | 8.15   | 128.17      | 119.78   |
| 17  | r     | 51  | VAL  | N-CA-C | -8.01  | 102.62      | 109.19   |
| 47  | W     | 69  | TYR  | N-CA-C | -7.74  | 102.78      | 111.14   |
| 41  | Q     | 114 | SER  | N-CA-C | -7.38  | 103.31      | 111.36   |
| 7   | h     | 44  | ALA  | N-CA-C | -7.37  | 102.94      | 112.23   |
| 38  | N     | 103 | VAL  | N-CA-C | -7.37  | 105.39      | 113.43   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | J     | 141  | ASP  | N-CA-C      | -7.37 | 103.33      | 111.36   |
| 1   | b     | 12   | ARG  | N-CA-C      | -7.21 | 105.02      | 114.31   |
| 46  | V     | 51   | GLU  | N-CA-C      | -7.13 | 103.68      | 112.88   |
| 35  | K     | 66   | ALA  | N-CA-C      | 7.11  | 114.61      | 108.22   |
| 29  | E     | 63   | TYR  | N-CA-C      | 6.80  | 118.35      | 111.07   |
| 36  | L     | 83   | THR  | N-CA-C      | 6.75  | 119.02      | 110.24   |
| 37  | M     | 28   | SER  | N-CA-C      | 6.73  | 119.01      | 110.33   |
| 46  | V     | 32   | ILE  | N-CA-C      | 6.69  | 117.32      | 111.90   |
| 3   | d     | 176  | ASP  | CA-C-N      | 6.67  | 126.17      | 119.24   |
| 3   | d     | 176  | ASP  | C-N-CA      | 6.67  | 126.17      | 119.24   |
| 42  | R     | 15   | VAL  | N-CA-C      | 6.48  | 116.64      | 110.42   |
| 13  | n     | 68   | ALA  | N-CA-C      | -6.43 | 104.27      | 111.28   |
| 8   | i     | 127  | SER  | N-CA-C      | -6.40 | 103.82      | 111.69   |
| 47  | W     | 17   | VAL  | N-CA-C      | 6.40  | 117.68      | 109.30   |
| 49  | Y     | 61   | ALA  | N-CA-C      | -6.40 | 104.40      | 111.82   |
| 45  | U     | 54   | LEU  | N-CA-C      | 6.39  | 121.91      | 111.37   |
| 36  | L     | 143  | MET  | N-CA-C      | -6.39 | 104.53      | 112.90   |
| 47  | W     | 60   | ARG  | N-CA-C      | -6.38 | 103.84      | 111.69   |
| 44  | T     | 43   | ALA  | N-CA-C      | -6.35 | 104.44      | 111.36   |
| 31  | G     | 92   | ASN  | N-CA-C      | 6.34  | 120.62      | 112.12   |
| 52  | 3     | 1190 | G    | C2'-C3'-O3' | 6.32  | 118.97      | 109.50   |
| 42  | R     | 78   | ARG  | N-CA-C      | -6.28 | 105.11      | 112.89   |
| 1   | b     | 131  | MET  | N-CA-C      | 6.22  | 120.33      | 112.87   |
| 19  | t     | 50   | LEU  | N-CA-C      | 6.22  | 118.14      | 111.36   |
| 41  | Q     | 110  | LYS  | N-CA-C      | 6.20  | 117.91      | 111.03   |
| 36  | L     | 16   | LYS  | N-CA-C      | -6.15 | 103.88      | 112.12   |
| 40  | P     | 125  | LYS  | N-CA-C      | 6.13  | 123.85      | 110.80   |
| 13  | n     | 60   | VAL  | N-CA-C      | -6.11 | 106.55      | 111.81   |
| 34  | J     | 105  | ILE  | N-CA-C      | 6.11  | 115.14      | 106.53   |
| 49  | Y     | 5    | SER  | N-CA-C      | -6.07 | 105.86      | 113.20   |
| 24  | y     | 24   | GLU  | N-CA-C      | 6.06  | 118.68      | 111.71   |
| 33  | I     | 166  | LYS  | CA-C-N      | 6.00  | 127.35      | 119.84   |
| 33  | I     | 166  | LYS  | C-N-CA      | 6.00  | 127.35      | 119.84   |
| 36  | L     | 120  | ALA  | N-CA-C      | -5.99 | 104.83      | 111.36   |
| 52  | 3     | 1201 | A    | C2'-C3'-O3' | 5.97  | 118.46      | 109.50   |
| 47  | W     | 12   | PHE  | N-CA-C      | 5.95  | 116.28      | 108.07   |
| 10  | k     | 32   | TYR  | N-CA-C      | 5.91  | 117.52      | 110.19   |
| 10  | k     | 95   | ILE  | N-CA-C      | 5.90  | 115.97      | 110.42   |
| 35  | K     | 68   | GLN  | N-CA-C      | 5.87  | 117.67      | 111.28   |
| 4   | e     | 109  | ARG  | N-CA-C      | 5.87  | 119.95      | 113.21   |
| 50  | Z     | 29   | ALA  | N-CA-C      | -5.86 | 106.76      | 112.97   |
| 13  | n     | 67   | PHE  | N-CA-C      | -5.84 | 106.28      | 113.41   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 28  | D     | 7    | PRO  | N-CA-C      | 5.78  | 120.41      | 111.21   |
| 16  | q     | 85   | ALA  | N-CA-C      | -5.77 | 106.10      | 114.12   |
| 7   | h     | 117  | LEU  | N-CA-C      | 5.74  | 118.08      | 108.73   |
| 3   | d     | 73   | ILE  | N-CA-C      | -5.68 | 104.61      | 112.50   |
| 45  | U     | 69   | ASP  | N-CA-C      | 5.65  | 117.11      | 111.07   |
| 49  | Y     | 7    | LYS  | N-CA-C      | -5.65 | 106.39      | 113.28   |
| 18  | s     | 40   | ASN  | N-CA-C      | 5.62  | 118.30      | 108.52   |
| 4   | e     | 174  | PHE  | CA-C-N      | 5.62  | 126.86      | 119.84   |
| 4   | e     | 174  | PHE  | C-N-CA      | 5.62  | 126.86      | 119.84   |
| 8   | i     | 24   | GLY  | CA-C-N      | 5.60  | 125.22      | 119.56   |
| 8   | i     | 24   | GLY  | C-N-CA      | 5.60  | 125.22      | 119.56   |
| 11  | l     | 95   | LEU  | N-CA-C      | -5.59 | 105.19      | 112.23   |
| 44  | T     | 53   | ARG  | N-CA-C      | -5.59 | 105.33      | 111.82   |
| 50  | Z     | 58   | LYS  | N-CA-C      | -5.59 | 105.27      | 111.36   |
| 34  | J     | 84   | VAL  | N-CA-C      | 5.58  | 117.03      | 108.71   |
| 44  | T     | 39   | GLN  | N-CA-C      | -5.58 | 105.35      | 111.82   |
| 4   | e     | 164  | GLU  | N-CA-C      | -5.58 | 106.31      | 113.23   |
| 23  | x     | 10   | ARG  | CA-C-N      | 5.55  | 126.78      | 119.84   |
| 23  | x     | 10   | ARG  | C-N-CA      | 5.55  | 126.78      | 119.84   |
| 42  | R     | 107  | THR  | N-CA-C      | -5.52 | 105.18      | 111.14   |
| 10  | k     | 89   | ASN  | N-CA-C      | 5.49  | 122.50      | 110.80   |
| 31  | G     | 162  | VAL  | N-CA-C      | 5.47  | 116.86      | 108.71   |
| 32  | H     | 5    | HIS  | CA-C-N      | 5.47  | 126.67      | 119.84   |
| 32  | H     | 5    | HIS  | C-N-CA      | 5.47  | 126.67      | 119.84   |
| 37  | M     | 55   | LYS  | CA-C-N      | 5.45  | 125.77      | 119.93   |
| 37  | M     | 55   | LYS  | C-N-CA      | 5.45  | 125.77      | 119.93   |
| 16  | q     | 103  | VAL  | N-CA-C      | -5.43 | 105.24      | 110.72   |
| 41  | Q     | 54   | VAL  | N-CA-C      | 5.41  | 115.92      | 108.12   |
| 53  | l     | 1020 | A    | C2'-C3'-O3' | 5.41  | 117.62      | 109.50   |
| 49  | Y     | 84   | LYS  | N-CA-C      | -5.39 | 106.20      | 112.89   |
| 10  | k     | 71   | ARG  | N-CA-C      | -5.39 | 103.28      | 110.07   |
| 32  | H     | 98   | ALA  | N-CA-C      | 5.35  | 117.62      | 108.90   |
| 44  | T     | 61   | GLN  | N-CA-C      | -5.33 | 105.55      | 111.36   |
| 32  | H     | 13   | ILE  | N-CA-C      | 5.31  | 115.82      | 111.62   |
| 3   | d     | 88   | ARG  | N-CA-C      | -5.28 | 103.49      | 110.40   |
| 9   | j     | 119  | PHE  | N-CA-C      | -5.27 | 106.70      | 113.23   |
| 35  | K     | 69   | GLU  | N-CA-C      | 5.25  | 116.81      | 111.14   |
| 2   | c     | 152  | PRO  | N-CA-C      | -5.25 | 106.37      | 113.40   |
| 42  | R     | 34   | ALA  | N-CA-C      | -5.24 | 105.24      | 111.69   |
| 43  | S     | 40   | ARG  | N-CA-C      | -5.23 | 105.75      | 111.82   |
| 18  | s     | 24   | ILE  | N-CA-C      | 5.23  | 117.14      | 112.17   |
| 32  | H     | 89   | VAL  | N-CA-C      | 5.22  | 119.39      | 112.76   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 18  | s     | 42   | LYS  | N-CA-C     | -5.21 | 105.78      | 111.82   |
| 11  | l     | 137  | ALA  | N-CA-C     | -5.19 | 106.46      | 112.89   |
| 40  | P     | 69   | CYS  | N-CA-C     | -5.18 | 107.00      | 113.38   |
| 43  | S     | 20   | PHE  | N-CA-C     | 5.17  | 117.36      | 110.53   |
| 52  | 3     | 1300 | G    | N9-C1'-C2' | 5.17  | 119.76      | 112.00   |
| 48  | X     | 3    | SER  | N-CA-C     | 5.16  | 116.36      | 108.52   |
| 40  | P     | 68   | ARG  | N-CA-C     | -5.14 | 106.51      | 112.89   |
| 38  | N     | 57   | VAL  | N-CA-C     | 5.14  | 120.03      | 109.34   |
| 34  | J     | 55   | VAL  | N-CA-C     | 5.14  | 119.98      | 108.88   |
| 5   | f     | 3    | VAL  | N-CA-C     | -5.12 | 107.42      | 113.42   |
| 14  | o     | 68   | LYS  | N-CA-C     | 5.11  | 117.24      | 111.11   |
| 52  | 3     | 1301 | U    | N1-C1'-C2' | 5.10  | 119.65      | 112.00   |
| 52  | 3     | 1225 | A    | N9-C1'-C2' | 5.09  | 119.64      | 112.00   |
| 30  | F     | 4    | ARG  | N-CA-C     | 5.09  | 116.50      | 110.19   |
| 30  | F     | 35   | GLN  | N-CA-C     | 5.09  | 115.00      | 108.34   |
| 31  | G     | 198  | VAL  | N-CA-C     | 5.08  | 116.85      | 108.97   |
| 4   | e     | 34   | THR  | N-CA-C     | 5.08  | 116.68      | 108.34   |
| 9   | j     | 79   | GLY  | N-CA-C     | -5.06 | 108.14      | 115.27   |
| 32  | H     | 8    | GLY  | N-CA-C     | 5.05  | 118.36      | 112.50   |
| 11  | l     | 55   | MET  | CA-C-N     | 5.05  | 126.16      | 119.84   |
| 11  | l     | 55   | MET  | C-N-CA     | 5.05  | 126.16      | 119.84   |
| 53  | l     | 1818 | U    | N1-C1'-C2' | 5.04  | 119.55      | 112.00   |
| 38  | N     | 60   | LEU  | N-CA-C     | 5.03  | 116.88      | 108.99   |
| 18  | s     | 38   | TYR  | N-CA-C     | 5.03  | 119.10      | 112.92   |
| 1   | b     | 11   | GLY  | N-CA-C     | -5.02 | 107.87      | 114.95   |
| 36  | L     | 142  | ARG  | N-CA-C     | -5.02 | 107.11      | 113.18   |
| 7   | h     | 30   | SER  | N-CA-C     | -5.02 | 106.08      | 113.61   |
| 2   | c     | 61   | THR  | N-CA-C     | 5.00  | 116.98      | 110.43   |
| 34  | J     | 122  | VAL  | N-CA-C     | 5.00  | 119.74      | 109.34   |

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     | 56      | 0            |
| 2   | c     | 1565  | 0        | 1616     | 34      | 0            |
| 3   | d     | 1552  | 0        | 1619     | 33      | 0            |
| 4   | e     | 1411  | 0        | 1447     | 41      | 0            |
| 5   | f     | 1323  | 0        | 1374     | 28      | 0            |
| 6   | g     | 1111  | 0        | 1148     | 31      | 0            |
| 7   | h     | 989   | 0        | 1025     | 38      | 0            |
| 8   | i     | 1032  | 0        | 1088     | 41      | 0            |
| 9   | j     | 1129  | 0        | 1162     | 25      | 0            |
| 10  | k     | 939   | 0        | 1012     | 25      | 0            |
| 11  | l     | 1045  | 0        | 1117     | 20      | 0            |
| 12  | m     | 1074  | 0        | 1157     | 29      | 0            |
| 13  | n     | 961   | 0        | 1000     | 26      | 0            |
| 14  | o     | 892   | 0        | 923      | 22      | 0            |
| 15  | p     | 917   | 0        | 965      | 31      | 0            |
| 16  | q     | 947   | 0        | 1022     | 19      | 0            |
| 17  | r     | 816   | 0        | 839      | 23      | 0            |
| 18  | s     | 857   | 0        | 922      | 25      | 0            |
| 19  | t     | 739   | 0        | 807      | 15      | 0            |
| 20  | u     | 780   | 0        | 834      | 19      | 0            |
| 21  | v     | 753   | 0        | 780      | 17      | 0            |
| 22  | w     | 575   | 0        | 592      | 8       | 0            |
| 23  | x     | 625   | 0        | 655      | 9       | 0            |
| 24  | y     | 509   | 0        | 543      | 14      | 0            |
| 25  | z     | 449   | 0        | 491      | 9       | 0            |
| 26  | B     | 444   | 0        | 461      | 13      | 0            |
| 27  | C     | 410   | 0        | 440      | 2       | 0            |
| 28  | D     | 377   | 0        | 418      | 8       | 0            |
| 29  | E     | 504   | 0        | 574      | 10      | 0            |
| 30  | F     | 302   | 0        | 343      | 13      | 0            |
| 31  | G     | 1757  | 0        | 1787     | 30      | 0            |
| 32  | H     | 1625  | 0        | 1699     | 35      | 0            |
| 33  | I     | 1643  | 0        | 1710     | 40      | 0            |
| 34  | J     | 1157  | 0        | 1199     | 25      | 0            |
| 35  | K     | 818   | 0        | 808      | 28      | 0            |
| 36  | L     | 1182  | 0        | 1240     | 43      | 0            |
| 37  | M     | 979   | 0        | 1034     | 22      | 0            |
| 38  | N     | 1022  | 0        | 1070     | 32      | 0            |
| 39  | O     | 787   | 0        | 828      | 26      | 0            |
| 40  | P     | 870   | 0        | 878      | 39      | 0            |
| 41  | Q     | 955   | 0        | 1019     | 36      | 0            |
| 42  | R     | 884   | 0        | 944      | 24      | 0            |
| 43  | S     | 805   | 0        | 847      | 30      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 44  | T     | 714    | 0        | 737      | 20      | 0            |
| 45  | U     | 649    | 0        | 666      | 22      | 0            |
| 46  | V     | 649    | 0        | 691      | 19      | 0            |
| 47  | W     | 536    | 0        | 552      | 11      | 0            |
| 48  | X     | 638    | 0        | 665      | 18      | 0            |
| 49  | Y     | 665    | 0        | 714      | 14      | 0            |
| 50  | Z     | 545    | 0        | 579      | 26      | 0            |
| 51  | a     | 1027   | 0        | 1092     | 26      | 0            |
| 52  | 3     | 33012  | 0        | 16618    | 355     | 0            |
| 53  | 1     | 62317  | 0        | 31346    | 669     | 0            |
| 54  | 2     | 2568   | 0        | 1303     | 44      | 0            |
| 55  | 5     | 1640   | 0        | 836      | 10      | 0            |
| 55  | 6     | 1640   | 0        | 837      | 11      | 0            |
| 56  | 4     | 388    | 0        | 197      | 1       | 0            |
| 57  | 7     | 1619   | 0        | 821      | 11      | 0            |
| 58  | 5     | 10     | 0        | 10       | 0       | 0            |
| 59  | 7     | 11     | 0        | 8        | 0       | 0            |
| All | All   | 150222 | 0        | 101266   | 2038    | 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 8.

All (2038) 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'    | 1.28                     | 1.15              |
| 8:i:25:PRO:HB2   | 53:1:1095:A:H61  | 1.12                     | 1.14              |
| 9:j:100:VAL:HG13 | 9:j:101:ILE:HD12 | 1.41                     | 1.00              |
| 8:i:91:LYS:HE2   | 8:i:91:LYS:HA    | 1.47                     | 0.94              |
| 12:m:12:MET:HA   | 53:1:910:A:H62   | 1.31                     | 0.94              |
| 40:P:125:LYS:HE2 | 50:Z:33:ARG:HE   | 1.32                     | 0.94              |
| 35:K:3:HIS:H     | 35:K:92:THR:HG22 | 1.32                     | 0.93              |
| 34:J:107:GLY:HA3 | 52:3:9:G:H5'     | 1.54                     | 0.89              |
| 50:Z:9:GLU:HB3   | 50:Z:10:PRO:HD3  | 1.50                     | 0.89              |
| 53:1:2277:G:H2'  | 53:1:2278:A:H5'' | 1.54                     | 0.89              |
| 8:i:25:PRO:HB2   | 53:1:1095:A:N6   | 1.87                     | 0.88              |
| 14:o:3:LYS:NZ    | 54:2:29:A:H5''   | 1.89                     | 0.86              |
| 48:X:77:ARG:HH21 | 52:3:1225:A:H4'  | 1.40                     | 0.85              |
| 7:h:55:VAL:HA    | 53:1:1084:A:H4'  | 1.56                     | 0.85              |
| 53:1:2286:G:H5'' | 53:1:2287:A:OP1  | 1.78                     | 0.84              |
| 1:b:106:PRO:HD2  | 1:b:109:LEU:HD22 | 1.59                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:3:484:G:H4'    | 52:3:485:U:H5''   | 1.61                     | 0.83              |
| 10:k:88:ASN:HD22  | 10:k:93:GLN:HG3   | 1.44                     | 0.83              |
| 53:1:1906:G:H2'   | 53:1:1907:G:H5''  | 1.59                     | 0.82              |
| 30:F:36:ARG:HG2   | 30:F:37:GLN:H     | 1.43                     | 0.82              |
| 7:h:43:LYS:HA     | 7:h:46:ARG:HG2    | 1.61                     | 0.82              |
| 15:p:102:ARG:HH22 | 53:1:1754:A:H4'   | 1.44                     | 0.82              |
| 5:f:169:ARG:HH12  | 53:1:1093:G:C5'   | 1.93                     | 0.81              |
| 53:1:821:A:H5''   | 53:1:822:G:H5''   | 1.63                     | 0.81              |
| 32:H:171:ARG:HG2  | 32:H:173:PRO:HD3  | 1.62                     | 0.80              |
| 52:3:1200:C:H5''  | 52:3:1201:A:H3'   | 1.62                     | 0.80              |
| 38:N:20:ILE:HD11  | 38:N:60:LEU:HD22  | 1.62                     | 0.80              |
| 52:3:1033:G:H2'   | 52:3:1034:G:H5''  | 1.64                     | 0.79              |
| 7:h:40:GLU:HA     | 7:h:43:LYS:HE2    | 1.65                     | 0.78              |
| 35:K:52:ASN:O     | 35:K:53:LYS:HB2   | 1.84                     | 0.78              |
| 54:2:3:C:H2'      | 54:2:4:C:H5''     | 1.63                     | 0.78              |
| 53:1:1053:C:H2'   | 53:1:1054:A:H5''  | 1.66                     | 0.77              |
| 45:U:78:VAL:O     | 45:U:79:ASN:HB2   | 1.85                     | 0.76              |
| 11:l:93:ASN:O     | 11:l:94:THR:HG22  | 1.85                     | 0.76              |
| 11:l:101:ILE:HG13 | 11:l:102:GLY:H    | 1.51                     | 0.76              |
| 54:2:88:C:H4'     | 54:2:89:U:OP1     | 1.86                     | 0.76              |
| 46:V:47:ASP:HB3   | 46:V:74:LEU:HD13  | 1.68                     | 0.76              |
| 34:J:108:GLY:H    | 52:3:9:G:H4'      | 1.51                     | 0.76              |
| 45:U:5:ARG:HB2    | 52:3:376:G:H5''   | 1.68                     | 0.76              |
| 18:s:6:LYS:HG2    | 53:1:494:G:H4'    | 1.69                     | 0.75              |
| 33:I:8:LEU:HB3    | 52:3:430:A:OP1    | 1.85                     | 0.75              |
| 45:U:33:ILE:HG22  | 45:U:34:GLU:HG2   | 1.66                     | 0.75              |
| 34:J:105:ILE:HD12 | 34:J:123:LEU:HD23 | 1.67                     | 0.75              |
| 2:c:151:THR:HB    | 2:c:152:PRO:HD3   | 1.69                     | 0.75              |
| 34:J:80:LEU:HG    | 34:J:122:VAL:HG11 | 1.67                     | 0.74              |
| 12:m:64:TRP:HB2   | 12:m:104:GLU:HB2  | 1.69                     | 0.74              |
| 31:G:112:ARG:HH22 | 52:3:1104:G:H4'   | 1.52                     | 0.74              |
| 53:1:1020:A:H1'   | 53:1:1021:A:OP2   | 1.87                     | 0.74              |
| 5:f:169:ARG:HH12  | 53:1:1093:G:H5''  | 1.51                     | 0.74              |
| 15:p:88:ARG:HE    | 15:p:112:ARG:HH21 | 1.35                     | 0.74              |
| 24:y:2:LYS:HE3    | 53:1:102:U:H1'    | 1.67                     | 0.74              |
| 52:3:1301:U:O2    | 52:3:1301:U:H2'   | 1.88                     | 0.74              |
| 49:Y:80:ALA:HA    | 49:Y:83:ASN:HD21  | 1.52                     | 0.73              |
| 20:u:84:PHE:HB2   | 53:1:297:G:H5''   | 1.69                     | 0.73              |
| 6:g:72:ILE:HB     | 6:g:108:VAL:HG12  | 1.71                     | 0.73              |
| 52:3:405:U:H3'    | 52:3:406:G:H5'    | 1.71                     | 0.73              |
| 53:1:2427:C:H5''  | 53:1:2429:G:H5'   | 1.71                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:n:2:ARG:O      | 13:n:2:ARG:HD3    | 1.89                     | 0.73              |
| 49:Y:3:ILE:H      | 49:Y:3:ILE:HD12   | 1.53                     | 0.73              |
| 1:b:16:VAL:HB     | 1:b:203:VAL:HG22  | 1.71                     | 0.73              |
| 35:K:44:ARG:HG2   | 35:K:56:LYS:HG3   | 1.70                     | 0.73              |
| 53:1:1900:A:H1'   | 53:1:1970:A:H2'   | 1.70                     | 0.72              |
| 52:3:149:A:H61    | 52:3:172:A:H62    | 1.36                     | 0.72              |
| 53:1:329:G:O4'    | 53:1:477:A:H1'    | 1.90                     | 0.72              |
| 7:h:59:LEU:HB3    | 7:h:62:ARG:HB2    | 1.71                     | 0.72              |
| 25:z:25:GLY:HA3   | 25:z:46:MET:HE1   | 1.72                     | 0.72              |
| 31:G:24:PRO:HB3   | 52:3:828:U:H2'    | 1.71                     | 0.72              |
| 37:M:45:ILE:HD13  | 37:M:60:LEU:HD22  | 1.72                     | 0.71              |
| 53:1:2277:G:C2'   | 53:1:2278:A:H5''  | 2.20                     | 0.71              |
| 53:1:2553:G:H3'   | 53:1:2554:U:H5''  | 1.71                     | 0.71              |
| 52:3:701:U:H4'    | 52:3:703:G:H1'    | 1.72                     | 0.71              |
| 8:i:133:ARG:HH22  | 53:1:1079:C:C4'   | 2.03                     | 0.71              |
| 36:L:55:LYS:HB3   | 36:L:59:GLU:HG3   | 1.73                     | 0.71              |
| 53:1:713:G:H21    | 53:1:718:A:H62    | 1.39                     | 0.71              |
| 8:i:12:VAL:HG13   | 53:1:1061:U:H3    | 1.56                     | 0.71              |
| 33:I:131:ILE:HG21 | 52:3:620:C:H1'    | 1.73                     | 0.71              |
| 53:1:275:C:H2'    | 53:1:276:U:H4'    | 1.73                     | 0.71              |
| 53:1:2391:G:H4'   | 53:1:2392:A:OP1   | 1.89                     | 0.71              |
| 4:e:40:GLY:HA2    | 4:e:84:ILE:HD11   | 1.72                     | 0.71              |
| 32:H:111:ASP:HB3  | 32:H:114:LEU:HB2  | 1.73                     | 0.70              |
| 35:K:23:GLU:HA    | 35:K:26:THR:HG22  | 1.73                     | 0.70              |
| 51:a:163:TYR:HB2  | 51:a:171:ILE:HD11 | 1.73                     | 0.70              |
| 2:c:156:PHE:HB3   | 9:j:81:ILE:HG22   | 1.73                     | 0.70              |
| 1:b:245:THR:HG23  | 1:b:247:TRP:H     | 1.56                     | 0.70              |
| 16:q:47:ARG:HH21  | 16:q:51:GLN:HE22  | 1.40                     | 0.70              |
| 32:H:78:LYS:O     | 32:H:79:LYS:HG3   | 1.91                     | 0.70              |
| 1:b:156:SER:HB2   | 53:1:1818:U:H5'   | 1.72                     | 0.70              |
| 52:3:1201:A:H1'   | 52:3:1202:U:OP2   | 1.90                     | 0.70              |
| 39:O:53:ILE:HG13  | 43:S:84:ARG:HD2   | 1.73                     | 0.70              |
| 10:k:108:ARG:HB3  | 10:k:116:ILE:HG21 | 1.74                     | 0.70              |
| 42:R:6:ILE:HG13   | 42:R:7:ASN:H      | 1.55                     | 0.70              |
| 34:J:92:ARG:HB2   | 34:J:127:TYR:HB2  | 1.74                     | 0.69              |
| 53:1:215:G:H4'    | 53:1:216:A:H4'    | 1.73                     | 0.69              |
| 4:e:88:VAL:HA     | 54:2:42:C:O2      | 1.92                     | 0.69              |
| 7:h:108:VAL:HG13  | 7:h:109:LYS:H     | 1.57                     | 0.69              |
| 47:W:59:LYS:HE2   | 52:3:735:C:H5'    | 1.73                     | 0.69              |
| 53:1:704:G:H2'    | 53:1:726:G:H22    | 1.57                     | 0.69              |
| 53:1:2128:G:H21   | 53:1:2173:A:H1'   | 1.57                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:k:110:GLU:H    | 10:k:113:MET:HE3  | 1.58                     | 0.69              |
| 31:G:163:ILE:HG23 | 31:G:185:ILE:HD11 | 1.74                     | 0.69              |
| 32:H:69:THR:HG21  | 32:H:75:VAL:HG21  | 1.74                     | 0.69              |
| 4:e:132:ARG:CZ    | 53:1:2305:U:H4'   | 2.23                     | 0.68              |
| 53:1:807:U:H2'    | 53:1:808:G:H8     | 1.58                     | 0.68              |
| 46:V:16:MET:HG3   | 46:V:19:SER:OG    | 1.93                     | 0.68              |
| 6:g:42:LYS:O      | 6:g:45:GLU:HG2    | 1.94                     | 0.68              |
| 2:c:149:ASN:HB3   | 53:1:2572:A:OP2   | 1.93                     | 0.68              |
| 41:Q:87:LYS:HD2   | 52:3:526:C:OP2    | 1.94                     | 0.68              |
| 33:I:119:HIS:ND1  | 52:3:438:U:H4'    | 2.09                     | 0.68              |
| 4:e:63:LYS:O      | 54:2:42:C:H1'     | 1.94                     | 0.68              |
| 37:M:29:SER:HB2   | 52:3:589:U:H5''   | 1.74                     | 0.68              |
| 39:O:57:VAL:O     | 39:O:58:ASN:HB2   | 1.94                     | 0.68              |
| 50:Z:9:GLU:HB3    | 50:Z:10:PRO:CD    | 2.24                     | 0.68              |
| 14:o:3:LYS:HZ2    | 54:2:29:A:H5''    | 1.57                     | 0.67              |
| 41:Q:49:ARG:HG3   | 41:Q:89:LEU:HD11  | 1.76                     | 0.67              |
| 35:K:3:HIS:N      | 35:K:92:THR:HG22  | 2.06                     | 0.67              |
| 53:1:45:G:H5''    | 53:1:46:G:C5'     | 2.17                     | 0.67              |
| 53:1:1133:A:H4'   | 53:1:1134:A:H5''  | 1.77                     | 0.67              |
| 53:1:1326:U:H2'   | 53:1:1327:A:H8    | 1.59                     | 0.67              |
| 2:c:33:ARG:HD3    | 2:c:73:VAL:HB     | 1.75                     | 0.67              |
| 4:e:116:LEU:H     | 4:e:175:PRO:HB2   | 1.60                     | 0.67              |
| 4:e:39:VAL:HG22   | 4:e:41:GLU:H      | 1.60                     | 0.67              |
| 13:n:39:PRO:HG2   | 53:1:1651:G:H4'   | 1.77                     | 0.67              |
| 39:O:10:LEU:HD23  | 39:O:10:LEU:H     | 1.60                     | 0.67              |
| 48:X:77:ARG:NH2   | 52:3:1225:A:H4'   | 2.09                     | 0.67              |
| 38:N:35:GLU:HA    | 38:N:39:GLY:HA3   | 1.77                     | 0.67              |
| 39:O:29:ALA:HB1   | 39:O:36:VAL:HG21  | 1.75                     | 0.67              |
| 45:U:31:ARG:HB2   | 52:3:310:G:H5''   | 1.77                     | 0.67              |
| 7:h:55:VAL:HA     | 53:1:1084:A:C4'   | 2.25                     | 0.66              |
| 52:3:1306:A:H61   | 52:3:1331:G:H1'   | 1.59                     | 0.66              |
| 1:b:164:VAL:HG21  | 1:b:180:MET:HE1   | 1.78                     | 0.66              |
| 14:o:90:VAL:HG12  | 14:o:91:SER:H     | 1.61                     | 0.66              |
| 6:g:112:LYS:HE2   | 53:1:2220:U:H5''  | 1.77                     | 0.66              |
| 7:h:61:ARG:HB3    | 53:1:1046:A:H4'   | 1.78                     | 0.66              |
| 24:y:8:GLU:HG2    | 24:y:12:GLU:HG2   | 1.77                     | 0.66              |
| 39:O:40:ILE:HB    | 39:O:73:LEU:HB3   | 1.77                     | 0.66              |
| 40:P:123:PRO:HG2  | 50:Z:33:ARG:CD    | 2.25                     | 0.66              |
| 46:V:11:VAL:HG22  | 46:V:20:ILE:HD11  | 1.78                     | 0.66              |
| 8:i:33:ASN:HD22   | 8:i:36:GLU:HG2    | 1.60                     | 0.66              |
| 18:s:79:GLY:H     | 18:s:101:SER:HA   | 1.61                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:V:26:ARG:NH2   | 52:3:237:G:H5''   | 2.11                     | 0.66              |
| 53:1:1186:G:H2'   | 53:1:1187:G:O4'   | 1.96                     | 0.66              |
| 12:m:13:HIS:HE1   | 53:1:2265:U:H4'   | 1.60                     | 0.66              |
| 36:L:75:LYS:HZ2   | 36:L:77:ARG:HB2   | 1.60                     | 0.66              |
| 52:3:327:A:O2'    | 52:3:328:C:H4'    | 1.96                     | 0.66              |
| 53:1:807:U:H2'    | 53:1:808:G:C8     | 2.30                     | 0.66              |
| 53:1:2296:U:H5''  | 53:1:2297:A:OP1   | 1.96                     | 0.66              |
| 4:e:141:ASP:H     | 4:e:144:LYS:HD3   | 1.61                     | 0.66              |
| 17:r:54:VAL:HG23  | 17:r:55:ASP:H     | 1.60                     | 0.66              |
| 53:1:1077:A:H2'   | 53:1:1078:U:H5'   | 1.78                     | 0.66              |
| 15:p:112:ARG:HG2  | 15:p:114:ASN:HD22 | 1.58                     | 0.66              |
| 52:3:463:U:H3     | 52:3:469:C:H42    | 1.42                     | 0.66              |
| 53:1:676:A:H62    | 53:1:802:A:H61    | 1.43                     | 0.66              |
| 53:1:1807:G:H2'   | 53:1:1808:A:H5'   | 1.78                     | 0.66              |
| 20:u:12:VAL:HA    | 20:u:69:VAL:HG12  | 1.78                     | 0.66              |
| 52:3:769:G:H4'    | 52:3:1513:A:H4'   | 1.78                     | 0.65              |
| 15:p:105:LYS:HD3  | 15:p:108:ARG:HH22 | 1.62                     | 0.65              |
| 19:t:29:THR:HG22  | 19:t:86:THR:HB    | 1.78                     | 0.65              |
| 33:I:8:LEU:HD22   | 52:3:429:U:H5'    | 1.78                     | 0.65              |
| 31:G:45:THR:HG22  | 31:G:200:PRO:HB2  | 1.79                     | 0.65              |
| 40:P:125:LYS:HE2  | 50:Z:33:ARG:NE    | 2.10                     | 0.65              |
| 53:1:281:C:H42    | 53:1:359:G:H1     | 1.44                     | 0.65              |
| 53:1:310:A:O2'    | 53:1:311:A:H5''   | 1.97                     | 0.65              |
| 7:h:55:VAL:HG12   | 53:1:1084:A:H4'   | 1.78                     | 0.65              |
| 54:2:3:C:C2'      | 54:2:4:C:H5''     | 2.27                     | 0.65              |
| 4:e:107:VAL:HG12  | 4:e:108:PRO:HD3   | 1.79                     | 0.65              |
| 38:N:54:VAL:HG12  | 38:N:93:LEU:HD11  | 1.77                     | 0.65              |
| 38:N:57:VAL:HG23  | 38:N:58:GLU:H     | 1.62                     | 0.65              |
| 52:3:1306:A:N6    | 52:3:1331:G:H1'   | 2.12                     | 0.65              |
| 40:P:118:ASN:HD22 | 52:3:718:A:H5'    | 1.61                     | 0.65              |
| 2:c:173:GLN:NE2   | 53:1:2772:C:H5'   | 2.11                     | 0.64              |
| 10:k:35:VAL:HG21  | 10:k:106:GLU:HB2  | 1.79                     | 0.64              |
| 34:J:12:GLU:HG2   | 34:J:38:VAL:HG12  | 1.78                     | 0.64              |
| 37:M:88:LYS:HE3   | 37:M:119:GLY:HA2  | 1.78                     | 0.64              |
| 31:G:103:TRP:HA   | 31:G:106:VAL:HG12 | 1.79                     | 0.64              |
| 9:j:7:LYS:HG2     | 53:1:538:A:H4'    | 1.78                     | 0.64              |
| 35:K:36:ILE:HA    | 35:K:64:VAL:HG23  | 1.79                     | 0.64              |
| 39:O:52:LEU:HD21  | 39:O:59:LYS:HD2   | 1.79                     | 0.64              |
| 53:1:161:A:H3'    | 53:1:162:U:H5''   | 1.78                     | 0.64              |
| 51:a:46:VAL:HG22  | 51:a:212:VAL:HG23 | 1.78                     | 0.64              |
| 3:d:158:PHE:HA    | 3:d:169:VAL:HG21  | 1.79                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 50:Z:66:ARG:HH21 | 52:3:1099:G:H4'   | 1.62                     | 0.64              |
| 53:1:2432:A:H1'  | 55:6:75:C:H5'     | 1.79                     | 0.64              |
| 10:k:35:VAL:HG13 | 10:k:36:GLY:H     | 1.63                     | 0.64              |
| 11:l:90:VAL:HG13 | 11:l:95:LEU:HD11  | 1.79                     | 0.64              |
| 9:j:81:ILE:HG13  | 9:j:82:GLY:H      | 1.63                     | 0.64              |
| 13:n:38:LEU:HB3  | 13:n:39:PRO:HD3   | 1.78                     | 0.64              |
| 22:w:39:THR:H    | 53:1:2331:G:H4'   | 1.62                     | 0.64              |
| 15:p:111:GLU:HB3 | 15:p:113:LEU:HD23 | 1.80                     | 0.64              |
| 20:u:85:ARG:HD3  | 20:u:87:GLU:HG3   | 1.78                     | 0.64              |
| 7:h:59:LEU:HD22  | 7:h:62:ARG:HH21   | 1.62                     | 0.64              |
| 42:R:102:LYS:HG3 | 52:3:1226:C:N4    | 2.12                     | 0.64              |
| 31:G:112:ARG:NH2 | 52:3:1104:G:H4'   | 2.13                     | 0.63              |
| 36:L:75:LYS:HE3  | 36:L:88:VAL:HG21  | 1.80                     | 0.63              |
| 52:3:1230:C:H5'  | 55:5:30:G:H5''    | 1.79                     | 0.63              |
| 18:s:83:LYS:HG2  | 18:s:95:ARG:HH11  | 1.63                     | 0.63              |
| 32:H:117:ASP:HA  | 32:H:120:THR:HG22 | 1.80                     | 0.63              |
| 3:d:77:ILE:HG13  | 3:d:78:TRP:HD1    | 1.63                     | 0.63              |
| 5:f:34:ARG:HE    | 5:f:70:LEU:HD13   | 1.62                     | 0.63              |
| 37:M:14:ARG:HD2  | 52:3:875:U:O2'    | 1.98                     | 0.63              |
| 53:1:2114:A:H61  | 53:1:2117:A:H62   | 1.45                     | 0.63              |
| 16:q:47:ARG:HH21 | 16:q:51:GLN:NE2   | 1.95                     | 0.63              |
| 53:1:704:G:H2'   | 53:1:726:G:N2     | 2.13                     | 0.63              |
| 53:1:2423:U:O2'  | 53:1:2425:A:H2'   | 1.98                     | 0.63              |
| 1:b:251:THR:HG23 | 1:b:252:LYS:HG2   | 1.80                     | 0.62              |
| 8:i:91:LYS:HB3   | 8:i:94:LYS:HB2    | 1.81                     | 0.62              |
| 22:w:21:ARG:HD2  | 22:w:25:GLU:HG2   | 1.82                     | 0.62              |
| 53:1:1045:C:H5'  | 53:1:1046:A:H5''  | 1.82                     | 0.62              |
| 6:g:6:LEU:HD11   | 6:g:37:VAL:HG23   | 1.82                     | 0.62              |
| 51:a:209:ILE:H   | 51:a:209:ILE:HD12 | 1.65                     | 0.62              |
| 53:1:995:C:H6    | 53:1:995:C:H5'    | 1.64                     | 0.62              |
| 53:1:644:A:H61   | 53:1:2349:G:H21   | 1.47                     | 0.62              |
| 6:g:116:ARG:HG3  | 6:g:133:GLN:HE22  | 1.65                     | 0.62              |
| 39:O:44:THR:HG23 | 39:O:69:THR:O     | 2.00                     | 0.62              |
| 23:x:63:ILE:H    | 23:x:63:ILE:HD12  | 1.65                     | 0.62              |
| 37:M:80:PRO:HG2  | 52:3:878:A:H5'    | 1.82                     | 0.62              |
| 8:i:77:VAL:HA    | 8:i:80:LYS:HD3    | 1.82                     | 0.62              |
| 12:m:105:MET:HE3 | 12:m:106:ASP:H    | 1.64                     | 0.62              |
| 53:1:1906:G:C2'  | 53:1:1907:G:H5''  | 2.28                     | 0.62              |
| 53:1:2286:G:H4'  | 53:1:2287:A:O4'   | 2.00                     | 0.61              |
| 13:n:7:GLY:HA3   | 53:1:2690:U:H3    | 1.64                     | 0.61              |
| 14:o:16:ARG:HD3  | 14:o:19:GLN:HE21  | 1.64                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:p:9:GLN:HA    | 15:p:12:MET:HB2   | 1.82                     | 0.61              |
| 53:1:996:A:H2'   | 53:1:997:G:H8     | 1.65                     | 0.61              |
| 53:1:2126:A:H2'  | 53:1:2162:G:H21   | 1.65                     | 0.61              |
| 2:c:12:THR:HG22  | 2:c:13:ARG:H      | 1.65                     | 0.61              |
| 16:q:82:LEU:HD12 | 16:q:87:VAL:HB    | 1.83                     | 0.61              |
| 36:L:139:ASP:O   | 36:L:143:MET:HG2  | 1.99                     | 0.61              |
| 52:3:1158:C:H2'  | 52:3:1159:U:H4'   | 1.82                     | 0.61              |
| 33:I:149:LYS:HG2 | 33:I:150:LYS:HG2  | 1.83                     | 0.61              |
| 36:L:12:LEU:HD12 | 36:L:13:PRO:HD2   | 1.83                     | 0.61              |
| 53:1:828:U:H2'   | 53:1:829:A:C8     | 2.35                     | 0.61              |
| 12:m:42:THR:HG22 | 12:m:93:VAL:HG12  | 1.81                     | 0.61              |
| 32:H:50:SER:HB2  | 32:H:114:LEU:HD11 | 1.81                     | 0.61              |
| 48:X:5:LYS:HE2   | 48:X:6:LYS:HE3    | 1.83                     | 0.61              |
| 53:1:2628:C:H3'  | 53:1:2629:U:H5'   | 1.82                     | 0.61              |
| 3:d:190:ALA:O    | 3:d:193:VAL:HG12  | 2.00                     | 0.61              |
| 5:f:174:LYS:O    | 5:f:175:LYS:HG3   | 2.00                     | 0.61              |
| 53:1:1141:U:H4'  | 53:1:1142:A:O4'   | 1.99                     | 0.61              |
| 49:Y:26:MET:HB3  | 52:3:1458:G:H5'   | 1.82                     | 0.61              |
| 38:N:51:LEU:HD21 | 38:N:82:ILE:HD13  | 1.83                     | 0.61              |
| 51:a:20:GLN:HA   | 51:a:223:ALA:HB3  | 1.83                     | 0.61              |
| 53:1:615:U:H5''  | 53:1:616:A:OP2    | 2.00                     | 0.61              |
| 53:1:2834:G:H2'  | 53:1:2879:A:H61   | 1.66                     | 0.61              |
| 8:i:21:PRO:HB2   | 8:i:22:PRO:HD3    | 1.81                     | 0.60              |
| 18:s:31:GLN:HA   | 18:s:34:ASP:OD1   | 2.01                     | 0.60              |
| 20:u:4:ILE:HD12  | 20:u:71:ILE:HG23  | 1.83                     | 0.60              |
| 42:R:76:ILE:HA   | 42:R:79:LEU:HD12  | 1.83                     | 0.60              |
| 8:i:90:GLY:O     | 8:i:91:LYS:HG2    | 2.02                     | 0.60              |
| 14:o:15:ARG:HD3  | 54:2:9:G:OP1      | 2.00                     | 0.60              |
| 2:c:109:VAL:HG21 | 2:c:193:VAL:HG12  | 1.82                     | 0.60              |
| 33:I:58:GLN:O    | 33:I:62:ARG:HD3   | 2.00                     | 0.60              |
| 33:I:69:ARG:O    | 33:I:72:ARG:HG2   | 2.01                     | 0.60              |
| 38:N:33:SER:H    | 38:N:36:GLN:HE21  | 1.47                     | 0.60              |
| 42:R:63:VAL:HG12 | 42:R:68:LEU:HG    | 1.83                     | 0.60              |
| 4:e:65:LEU:HD22  | 54:2:42:C:C5      | 2.37                     | 0.60              |
| 20:u:24:VAL:HG13 | 20:u:33:VAL:HG23  | 1.83                     | 0.60              |
| 51:a:27:ILE:HD12 | 51:a:182:ALA:HB1  | 1.83                     | 0.60              |
| 52:3:730:G:H2'   | 52:3:731:G:H5'    | 1.82                     | 0.60              |
| 13:n:100:CYS:HA  | 26:B:42:ILE:HG12  | 1.84                     | 0.60              |
| 17:r:15:SER:H    | 17:r:18:GLN:HE21  | 1.50                     | 0.60              |
| 53:1:1645:G:H5'' | 53:1:1646:C:H5'   | 1.83                     | 0.60              |
| 5:f:26:LYS:HB2   | 5:f:31:GLU:HG3    | 1.82                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:h:57:ASN:HB3   | 7:h:62:ARG:HD2    | 1.83                     | 0.60              |
| 30:F:13:ASN:HD22 | 30:F:29:ALA:HB2   | 1.66                     | 0.60              |
| 35:K:47:LEU:HD21 | 35:K:57:ALA:HB3   | 1.84                     | 0.60              |
| 40:P:125:LYS:HD2 | 52:3:797:C:OP1    | 2.01                     | 0.60              |
| 53:1:511:U:H2'   | 53:1:512:G:H5'    | 1.83                     | 0.60              |
| 31:G:162:VAL:HB  | 31:G:184:ALA:HB2  | 1.84                     | 0.60              |
| 53:1:1053:C:C2'  | 53:1:1054:A:H5''  | 2.31                     | 0.60              |
| 54:2:51:G:H2'    | 54:2:52:A:O4'     | 2.02                     | 0.60              |
| 57:7:43:C:H2'    | 57:7:44:G:C8      | 2.37                     | 0.60              |
| 17:r:51:VAL:HG22 | 17:r:52:PRO:HD2   | 1.82                     | 0.60              |
| 5:f:163:TYR:HB2  | 5:f:166:GLU:HB2   | 1.84                     | 0.59              |
| 5:f:169:ARG:HH12 | 53:1:1093:G:H5'   | 1.64                     | 0.59              |
| 7:h:117:LEU:O    | 7:h:118:ILE:HG12  | 2.02                     | 0.59              |
| 30:F:32:LYS:HE3  | 53:1:2478:A:H5'   | 1.84                     | 0.59              |
| 41:Q:79:ILE:HG22 | 41:Q:103:CYS:HB2  | 1.83                     | 0.59              |
| 15:p:38:ARG:HH22 | 15:p:40:GLN:HB3   | 1.67                     | 0.59              |
| 33:I:1:ALA:HA    | 33:I:67:LEU:HD11  | 1.85                     | 0.59              |
| 41:Q:71:HIS:HB2  | 41:Q:73:LEU:HD13  | 1.84                     | 0.59              |
| 34:J:10:LEU:HD23 | 34:J:10:LEU:H     | 1.67                     | 0.59              |
| 41:Q:120:ARG:CZ  | 52:3:500:G:H5'    | 2.32                     | 0.59              |
| 53:1:310:A:C2'   | 53:1:311:A:H5''   | 2.32                     | 0.59              |
| 9:j:81:ILE:HG13  | 9:j:82:GLY:N      | 2.18                     | 0.59              |
| 10:k:71:ARG:HD2  | 10:k:77:ILE:HD11  | 1.83                     | 0.59              |
| 40:P:123:PRO:HG2 | 50:Z:33:ARG:NE    | 2.18                     | 0.59              |
| 52:3:1497:G:O2'  | 52:3:1498:U:H5'   | 2.02                     | 0.59              |
| 53:1:189:G:H2'   | 53:1:205:G:H22    | 1.66                     | 0.59              |
| 20:u:16:LYS:HG3  | 53:1:329:G:H1     | 1.66                     | 0.59              |
| 30:F:19:ARG:HB2  | 30:F:24:ARG:HD2   | 1.84                     | 0.59              |
| 6:g:9:VAL:N      | 6:g:13:GLY:HA3    | 2.18                     | 0.59              |
| 8:i:126:ARG:HA   | 8:i:129:GLU:HG2   | 1.84                     | 0.59              |
| 15:p:105:LYS:HD3 | 15:p:108:ARG:HH12 | 1.66                     | 0.59              |
| 2:c:142:VAL:HG13 | 2:c:143:PRO:HD2   | 1.85                     | 0.59              |
| 45:U:14:ARG:HD2  | 45:U:42:ILE:HD13  | 1.85                     | 0.59              |
| 48:X:30:LEU:HB2  | 48:X:48:ILE:HG13  | 1.84                     | 0.59              |
| 24:y:22:LEU:HG   | 24:y:23:ARG:HD2   | 1.84                     | 0.59              |
| 31:G:26:MET:HE2  | 31:G:192:PRO:HD3  | 1.84                     | 0.59              |
| 36:L:24:LYS:HD2  | 52:3:1375:A:H5''  | 1.83                     | 0.59              |
| 10:k:1:MET:HG3   | 10:k:32:TYR:HB3   | 1.85                     | 0.59              |
| 12:m:41:LEU:HG   | 12:m:96:ILE:HG13  | 1.84                     | 0.59              |
| 37:M:77:VAL:HG23 | 37:M:126:CYS:HA   | 1.85                     | 0.59              |
| 50:Z:38:GLU:HB2  | 52:3:1526:G:OP2   | 2.03                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 53:1:2086:U:H2'   | 53:1:2087:G:C8   | 2.38                     | 0.59              |
| 53:1:2452:C:H42   | 53:1:2504:U:H3   | 1.51                     | 0.59              |
| 51:a:58:ASN:ND2   | 51:a:60:ARG:HD2  | 2.18                     | 0.58              |
| 52:3:70:U:H4'     | 52:3:71:A:H8     | 1.68                     | 0.58              |
| 53:1:1509:A:H2'   | 53:1:1510:G:C8   | 2.38                     | 0.58              |
| 8:i:11:GLN:HE22   | 8:i:58:ILE:HG12  | 1.67                     | 0.58              |
| 53:1:1105:U:H2'   | 53:1:1106:G:H5'' | 1.85                     | 0.58              |
| 14:o:15:ARG:HD3   | 54:2:9:G:P       | 2.42                     | 0.58              |
| 52:3:151:A:H62    | 52:3:170:U:H3    | 1.50                     | 0.58              |
| 3:d:63:LYS:HD2    | 53:1:2444:G:OP2  | 2.03                     | 0.58              |
| 52:3:1205:U:H2'   | 52:3:1206:G:H8   | 1.69                     | 0.58              |
| 53:1:473:G:O2'    | 53:1:474:G:H5'   | 2.03                     | 0.58              |
| 53:1:534:U:H2'    | 53:1:535:G:H8    | 1.69                     | 0.58              |
| 53:1:792:A:H3'    | 53:1:793:A:H5'   | 1.84                     | 0.58              |
| 7:h:81:LEU:HD21   | 53:1:1106:G:H21  | 1.67                     | 0.58              |
| 33:I:97:LEU:HB2   | 33:I:134:TYR:HB3 | 1.85                     | 0.58              |
| 38:N:51:LEU:HD12  | 38:N:56:MET:HB2  | 1.86                     | 0.58              |
| 40:P:72:ALA:H     | 40:P:74:LYS:HZ1  | 1.50                     | 0.58              |
| 51:a:37:LYS:HB2   | 53:1:2127:G:H5'  | 1.85                     | 0.58              |
| 53:1:1796:U:H2'   | 53:1:1797:G:H8   | 1.67                     | 0.58              |
| 6:g:26:ALA:HA     | 6:g:30:LEU:HB2   | 1.86                     | 0.58              |
| 41:Q:85:ARG:HH21  | 41:Q:87:LYS:HA   | 1.68                     | 0.58              |
| 52:3:225:C:H2'    | 52:3:226:G:H5''  | 1.86                     | 0.58              |
| 52:3:1219:A:H2'   | 52:3:1220:G:C8   | 2.39                     | 0.58              |
| 34:J:18:ASN:O     | 34:J:33:THR:HG22 | 2.02                     | 0.58              |
| 53:1:1373:A:H5'   | 53:1:2212:A:H1'  | 1.83                     | 0.58              |
| 22:w:36:GLN:NE2   | 22:w:39:THR:HA   | 2.18                     | 0.58              |
| 35:K:3:HIS:HA     | 35:K:65:GLU:HA   | 1.86                     | 0.58              |
| 53:1:1415:U:H2'   | 53:1:1416:G:H4'  | 1.86                     | 0.58              |
| 2:c:108:ASP:OD2   | 2:c:206:ALA:HA   | 2.04                     | 0.58              |
| 21:v:75:GLN:HB2   | 21:v:92:VAL:HG23 | 1.86                     | 0.58              |
| 57:7:44:G:H2'     | 57:7:45:U:O4'    | 2.04                     | 0.58              |
| 1:b:244:VAL:HG12  | 1:b:250:GLN:HA   | 1.85                     | 0.57              |
| 12:m:12:MET:HA    | 53:1:910:A:N6    | 2.11                     | 0.57              |
| 13:n:47:VAL:C     | 13:n:50:PRO:HD2  | 2.29                     | 0.57              |
| 48:X:54:ARG:HG3   | 48:X:55:GLN:HG3  | 1.84                     | 0.57              |
| 7:h:48:ALA:HB3    | 7:h:51:TYR:CE1   | 2.39                     | 0.57              |
| 7:h:58:THR:HA     | 7:h:63:ALA:HB3   | 1.86                     | 0.57              |
| 25:z:40:THR:HG23  | 25:z:43:ILE:H    | 1.70                     | 0.57              |
| 33:I:127:ARG:HH21 | 52:3:619:U:H4'   | 1.69                     | 0.57              |
| 33:I:150:LYS:HD3  | 33:I:177:MET:HE3 | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 46:V:49:ASN:CG   | 46:V:50:ASN:H    | 2.13                     | 0.57              |
| 52:3:410:G:H2'   | 52:3:429:U:C4    | 2.39                     | 0.57              |
| 53:1:2533:U:H2'  | 53:1:2534:A:O4'  | 2.04                     | 0.57              |
| 1:b:245:THR:OG1  | 1:b:246:PRO:HD2  | 2.05                     | 0.57              |
| 35:K:51:ILE:C    | 35:K:53:LYS:H    | 2.11                     | 0.57              |
| 53:1:1796:U:H2'  | 53:1:1797:G:C8   | 2.40                     | 0.57              |
| 57:7:9:A:H1'     | 57:7:45:U:O2'    | 2.04                     | 0.57              |
| 4:e:32:LYS:HD3   | 4:e:91:ARG:NH1   | 2.20                     | 0.57              |
| 50:Z:17:ARG:HA   | 50:Z:20:ARG:HG2  | 1.87                     | 0.57              |
| 5:f:136:ASP:HB3  | 5:f:139:VAL:HG22 | 1.86                     | 0.57              |
| 48:X:45:GLY:H    | 48:X:61:VAL:HG13 | 1.69                     | 0.57              |
| 53:1:1936:A:H2   | 53:1:1943:U:H3   | 1.50                     | 0.57              |
| 3:d:71:GLY:N     | 53:1:674:G:H5''  | 2.19                     | 0.57              |
| 15:p:4:ILE:O     | 15:p:8:GLU:HG2   | 2.05                     | 0.57              |
| 15:p:51:ASN:O    | 53:1:2845:U:H5'' | 2.05                     | 0.57              |
| 42:R:6:ILE:HG13  | 42:R:7:ASN:N     | 2.20                     | 0.57              |
| 45:U:51:ARG:C    | 45:U:52:LEU:HD22 | 2.30                     | 0.57              |
| 53:1:503:A:H4'   | 53:1:505:A:H5''  | 1.86                     | 0.57              |
| 44:T:30:LEU:HD21 | 52:3:658:C:H5'   | 1.86                     | 0.57              |
| 53:1:119:A:H4'   | 53:1:120:U:H5'   | 1.86                     | 0.57              |
| 12:m:69:PRO:HA   | 12:m:94:ALA:HB2  | 1.87                     | 0.57              |
| 53:1:441:U:O2'   | 53:1:442:G:H5'   | 2.04                     | 0.57              |
| 53:1:2029:G:O6   | 53:1:2032:G:H5'' | 2.04                     | 0.57              |
| 40:P:23:HIS:HB3  | 40:P:30:ILE:HG23 | 1.87                     | 0.57              |
| 54:2:3:C:C3'     | 54:2:4:C:H5''    | 2.35                     | 0.57              |
| 2:c:148:GLN:HB2  | 2:c:152:PRO:HG2  | 1.85                     | 0.56              |
| 6:g:63:ALA:HA    | 6:g:66:ASN:HD22  | 1.70                     | 0.56              |
| 8:i:12:VAL:HG13  | 53:1:1061:U:N3   | 2.19                     | 0.56              |
| 8:i:23:VAL:HG12  | 8:i:26:ALA:HB3   | 1.87                     | 0.56              |
| 14:o:76:LYS:O    | 14:o:80:GLU:HG3  | 2.05                     | 0.56              |
| 21:v:72:VAL:HG12 | 21:v:93:ARG:HA   | 1.87                     | 0.56              |
| 35:K:38:ARG:HG3  | 35:K:40:GLU:H    | 1.69                     | 0.56              |
| 40:P:88:PRO:HG2  | 40:P:89:GLY:H    | 1.70                     | 0.56              |
| 53:1:2646:C:H2'  | 53:1:2647:U:O4'  | 2.05                     | 0.56              |
| 3:d:109:LEU:HD23 | 3:d:112:LEU:HD12 | 1.86                     | 0.56              |
| 9:j:2:LYS:HB3    | 53:1:995:C:H42   | 1.70                     | 0.56              |
| 11:l:19:LEU:HD23 | 11:l:27:LEU:HD13 | 1.86                     | 0.56              |
| 47:W:59:LYS:HD2  | 52:3:734:G:O2'   | 2.05                     | 0.56              |
| 53:1:2360:G:H2'  | 53:1:2361:G:H5'  | 1.86                     | 0.56              |
| 4:e:24:VAL:HG12  | 54:2:55:U:H4'    | 1.87                     | 0.56              |
| 4:e:107:VAL:CG1  | 4:e:108:PRO:HD3  | 2.35                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:m:73:ILE:HG22 | 12:m:91:TYR:O     | 2.06                     | 0.56              |
| 14:o:81:ARG:O    | 14:o:84:GLU:HG3   | 2.05                     | 0.56              |
| 52:3:1219:A:H2'  | 52:3:1220:G:H8    | 1.70                     | 0.56              |
| 53:1:579:G:H4'   | 53:1:2018:G:H5''  | 1.88                     | 0.56              |
| 53:1:669:G:H2'   | 53:1:669:G:N3     | 2.20                     | 0.56              |
| 5:f:2:ARG:HH12   | 53:1:1113:U:H5'   | 1.70                     | 0.56              |
| 7:h:5:LEU:O      | 7:h:9:GLN:HG2     | 2.05                     | 0.56              |
| 8:i:133:ARG:NH2  | 53:1:1079:C:H4'   | 2.20                     | 0.56              |
| 10:k:48:PRO:HG3  | 52:3:1422:G:H5'   | 1.86                     | 0.56              |
| 11:l:132:ARG:HG3 | 11:l:142:ILE:HD12 | 1.86                     | 0.56              |
| 16:q:14:LYS:O    | 16:q:18:LYS:HG2   | 2.05                     | 0.56              |
| 16:q:23:TYR:CD1  | 53:1:533:G:H5'    | 2.40                     | 0.56              |
| 2:c:56:LYS:HE2   | 2:c:58:ASN:HD21   | 1.69                     | 0.56              |
| 7:h:30:SER:HB3   | 7:h:109:LYS:NZ    | 2.20                     | 0.56              |
| 52:3:501:C:H2'   | 52:3:502:A:C8     | 2.41                     | 0.56              |
| 53:1:112:U:H2'   | 53:1:113:U:H5'    | 1.88                     | 0.56              |
| 53:1:1476:U:H3   | 53:1:1515:A:H62   | 1.54                     | 0.56              |
| 15:p:51:ASN:C    | 15:p:52:ARG:HD2   | 2.31                     | 0.56              |
| 36:L:115:MET:HE3 | 36:L:118:ARG:HB2  | 1.88                     | 0.56              |
| 52:3:1346:A:H2'  | 52:3:1347:G:H4'   | 1.88                     | 0.56              |
| 9:j:25:LEU:HB3   | 53:1:1140:C:OP1   | 2.05                     | 0.56              |
| 34:J:148:SER:OG  | 34:J:151:MET:HG2  | 2.05                     | 0.56              |
| 52:3:1402:C:H2'  | 52:3:1403:C:O4'   | 2.05                     | 0.56              |
| 53:1:2480:C:H2'  | 53:1:2481:G:O4'   | 2.06                     | 0.56              |
| 1:b:239:PHE:HE2  | 1:b:243:PRO:HG3   | 1.71                     | 0.56              |
| 52:3:673:A:H2'   | 52:3:674:G:C8     | 2.41                     | 0.56              |
| 53:1:2800:A:H3'  | 53:1:2801:G:H5'   | 1.88                     | 0.56              |
| 20:u:32:LYS:NZ   | 53:1:478:A:H4'    | 2.20                     | 0.56              |
| 24:y:2:LYS:HD2   | 53:1:78:U:OP2     | 2.06                     | 0.56              |
| 29:E:31:ILE:HG23 | 29:E:31:ILE:O     | 2.06                     | 0.56              |
| 39:O:37:ARG:HH21 | 39:O:77:VAL:HG11  | 1.70                     | 0.56              |
| 40:P:72:ALA:H    | 40:P:74:LYS:NZ    | 2.04                     | 0.56              |
| 52:3:31:G:N2     | 52:3:47:C:H5''    | 2.21                     | 0.56              |
| 53:1:2287:A:O2'  | 53:1:2288:A:H2'   | 2.06                     | 0.56              |
| 12:m:1:MET:N     | 12:m:47:GLU:HG3   | 2.21                     | 0.56              |
| 33:I:18:LEU:HB3  | 33:I:63:ILE:HG22  | 1.88                     | 0.56              |
| 36:L:23:ALA:O    | 36:L:26:VAL:HG12  | 2.06                     | 0.56              |
| 41:Q:25:ALA:HA   | 52:3:554:A:H5'    | 1.87                     | 0.56              |
| 43:S:3:GLN:HA    | 43:S:6:LYS:HG3    | 1.88                     | 0.56              |
| 44:T:7:THR:O     | 44:T:11:VAL:HG23  | 2.05                     | 0.56              |
| 52:3:494:G:O2'   | 52:3:496:A:H1'    | 2.05                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:346:A:H2'   | 53:1:346:A:N3     | 2.21                     | 0.56              |
| 1:b:43:ASN:HD21  | 1:b:45:ASN:HB2    | 1.71                     | 0.55              |
| 13:n:29:VAL:HG21 | 13:n:75:ILE:HG23  | 1.88                     | 0.55              |
| 43:S:62:ARG:HG2  | 43:S:69:PRO:HA    | 1.88                     | 0.55              |
| 52:3:1197:A:H2'  | 52:3:1198:G:H5''  | 1.86                     | 0.55              |
| 53:1:49:A:H5'    | 53:1:51:G:O4'     | 2.06                     | 0.55              |
| 53:1:2508:G:H1   | 53:1:2580:U:H3    | 1.53                     | 0.55              |
| 3:d:143:LEU:HD11 | 3:d:185:LYS:HB2   | 1.88                     | 0.55              |
| 8:i:93:ASN:OD1   | 8:i:94:LYS:HD2    | 2.05                     | 0.55              |
| 19:t:69:ARG:HH22 | 53:1:1334:G:H5''  | 1.70                     | 0.55              |
| 53:1:1357:C:H2'  | 53:1:1358:G:O4'   | 2.07                     | 0.55              |
| 53:1:1827:U:O2'  | 53:1:1828:G:H5'   | 2.07                     | 0.55              |
| 53:1:2126:A:H2'  | 53:1:2162:G:N2    | 2.21                     | 0.55              |
| 55:5:6:G:O2'     | 55:5:7:G:H5'      | 2.06                     | 0.55              |
| 15:p:91:VAL:HG21 | 15:p:96:LEU:HD11  | 1.88                     | 0.55              |
| 35:K:3:HIS:HB2   | 35:K:92:THR:HA    | 1.87                     | 0.55              |
| 43:S:46:LYS:HA   | 43:S:49:THR:HG23  | 1.88                     | 0.55              |
| 53:1:215:G:C4'   | 53:1:216:A:H4'    | 2.37                     | 0.55              |
| 53:1:226:A:H2'   | 53:1:227:A:O4'    | 2.07                     | 0.55              |
| 2:c:62:LYS:HB2   | 2:c:63:PRO:HD3    | 1.88                     | 0.55              |
| 8:i:36:GLU:O     | 8:i:39:LYS:HG2    | 2.05                     | 0.55              |
| 35:K:10:VAL:HG12 | 35:K:58:HIS:HB3   | 1.87                     | 0.55              |
| 54:2:13:G:H21    | 54:2:16:G:H1'     | 1.71                     | 0.55              |
| 43:S:20:PHE:O    | 43:S:21:ALA:HB3   | 2.07                     | 0.55              |
| 53:1:2350:C:H2'  | 53:1:2351:G:O4'   | 2.05                     | 0.55              |
| 22:w:33:ILE:HG22 | 22:w:34:VAL:HG23  | 1.88                     | 0.55              |
| 37:M:77:VAL:HG12 | 37:M:84:ILE:HD12  | 1.89                     | 0.55              |
| 49:Y:56:ILE:HD13 | 49:Y:59:ARG:HH12  | 1.71                     | 0.55              |
| 52:3:1033:G:C2'  | 52:3:1034:G:H5''  | 2.35                     | 0.55              |
| 52:3:1230:C:H2'  | 52:3:1231:G:H8    | 1.72                     | 0.55              |
| 53:1:414:C:H2'   | 53:1:415:A:C8     | 2.42                     | 0.55              |
| 28:D:9:VAL:HG12  | 53:1:1309:G:OP1   | 2.07                     | 0.55              |
| 36:L:3:ARG:HB2   | 52:3:932:C:OP1    | 2.07                     | 0.55              |
| 41:Q:98:ARG:HB2  | 41:Q:116:TYR:HA   | 1.87                     | 0.55              |
| 52:3:392:C:H2'   | 52:3:393:A:C8     | 2.42                     | 0.55              |
| 52:3:501:C:H2'   | 52:3:502:A:H8     | 1.72                     | 0.55              |
| 53:1:2030:A:N3   | 53:1:2499:C:H5''  | 2.22                     | 0.55              |
| 8:i:94:LYS:HZ3   | 53:1:1076:C:H4'   | 1.72                     | 0.55              |
| 11:l:110:VAL:HB  | 11:l:127:VAL:HG23 | 1.88                     | 0.55              |
| 18:s:90:LYS:HB2  | 18:s:92:ARG:NH1   | 2.22                     | 0.55              |
| 31:G:27:LYS:HB3  | 31:G:28:PRO:HD3   | 1.89                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 41:Q:115:LYS:HG3  | 41:Q:116:TYR:CD2 | 2.41                     | 0.55              |
| 52:3:70:U:H4'     | 52:3:71:A:C8     | 2.42                     | 0.55              |
| 7:h:108:VAL:HG13  | 7:h:109:LYS:N    | 2.22                     | 0.55              |
| 32:H:40:GLN:O     | 32:H:44:LYS:HG2  | 2.06                     | 0.55              |
| 38:N:29:ILE:HG22  | 38:N:64:ILE:HB   | 1.89                     | 0.55              |
| 52:3:245:U:O2'    | 52:3:246:A:H5'   | 2.07                     | 0.55              |
| 52:3:1506:U:O2'   | 52:3:1507:A:H5'  | 2.07                     | 0.55              |
| 53:1:1049:C:H41   | 53:1:1110:G:H21  | 1.55                     | 0.55              |
| 7:h:94:ARG:HD3    | 7:h:94:ARG:N     | 2.23                     | 0.54              |
| 16:q:111:LYS:HB2  | 17:r:48:LYS:NZ   | 2.22                     | 0.54              |
| 28:D:24:THR:HG23  | 28:D:27:GLY:H    | 1.72                     | 0.54              |
| 52:3:29:U:O2'     | 52:3:30:U:H5'    | 2.07                     | 0.54              |
| 52:3:763:G:H2'    | 52:3:764:C:C6    | 2.42                     | 0.54              |
| 3:d:102:ARG:NH1   | 3:d:201:ALA:HB3  | 2.23                     | 0.54              |
| 10:k:21:CYS:HA    | 10:k:41:ILE:HG22 | 1.90                     | 0.54              |
| 31:G:96:LEU:H     | 31:G:96:LEU:HD12 | 1.72                     | 0.54              |
| 45:U:20:VAL:HG23  | 45:U:35:ARG:HA   | 1.89                     | 0.54              |
| 52:3:483:C:H2'    | 52:3:484:G:C8    | 2.42                     | 0.54              |
| 52:3:1218:C:H2'   | 52:3:1219:A:C8   | 2.43                     | 0.54              |
| 12:m:33:LEU:HD13  | 12:m:117:PHE:HB3 | 1.90                     | 0.54              |
| 17:r:68:ARG:HH11  | 17:r:90:ARG:HB2  | 1.72                     | 0.54              |
| 42:R:63:VAL:HG13  | 42:R:67:ASP:HB3  | 1.88                     | 0.54              |
| 23:x:18:SER:OG    | 53:1:2080:A:H5'  | 2.07                     | 0.54              |
| 31:G:185:ILE:HG13 | 31:G:185:ILE:O   | 2.07                     | 0.54              |
| 42:R:89:ARG:HG3   | 42:R:96:VAL:HA   | 1.89                     | 0.54              |
| 46:V:61:ARG:HD3   | 46:V:75:VAL:HG22 | 1.88                     | 0.54              |
| 52:3:77:A:H2'     | 52:3:78:A:C8     | 2.43                     | 0.54              |
| 12:m:1:MET:H2     | 12:m:47:GLU:HG3  | 1.73                     | 0.54              |
| 44:T:44:GLU:O     | 44:T:45:HIS:HB2  | 2.07                     | 0.54              |
| 53:1:2584:U:H2'   | 53:1:2585:U:H2'  | 1.89                     | 0.54              |
| 1:b:106:PRO:HG2   | 1:b:109:LEU:HB2  | 1.88                     | 0.54              |
| 5:f:8:VAL:HB      | 5:f:49:LEU:HB2   | 1.90                     | 0.54              |
| 43:S:63:CYS:HB3   | 43:S:67:GLY:H    | 1.72                     | 0.54              |
| 43:S:81:ILE:HG21  | 52:3:1202:U:N3   | 2.21                     | 0.54              |
| 53:1:996:A:H2'    | 53:1:997:G:C8    | 2.43                     | 0.54              |
| 53:1:1111:A:O2'   | 53:1:1112:G:H4'  | 2.07                     | 0.54              |
| 14:o:3:LYS:HZ1    | 54:2:29:A:H5''   | 1.69                     | 0.54              |
| 38:N:91:GLU:HA    | 38:N:94:ARG:HB2  | 1.88                     | 0.54              |
| 53:1:1105:U:C2'   | 53:1:1106:G:H5'' | 2.38                     | 0.54              |
| 53:1:1420:A:H5'   | 53:1:1421:G:OP2  | 2.08                     | 0.54              |
| 53:1:2055:C:H5'   | 53:1:2056:G:O5'  | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:1:2197:U:H1'  | 53:1:2198:A:C8   | 2.43                     | 0.54              |
| 3:d:79:ARG:HH21  | 53:1:448:U:H4'   | 1.73                     | 0.54              |
| 7:h:45:GLY:HA2   | 7:h:49:GLY:HA2   | 1.89                     | 0.54              |
| 32:H:1:GLY:HA2   | 52:3:1060:U:C5   | 2.43                     | 0.54              |
| 52:3:437:U:H2'   | 52:3:438:U:O4'   | 2.08                     | 0.54              |
| 52:3:1464:U:H2'  | 52:3:1465:A:C8   | 2.42                     | 0.54              |
| 5:f:148:ARG:HH11 | 5:f:152:ARG:HH21 | 1.54                     | 0.54              |
| 21:v:6:ALA:HB1   | 21:v:40:ILE:HG23 | 1.89                     | 0.54              |
| 50:Z:16:ARG:HB2  | 50:Z:19:LYS:HE2  | 1.89                     | 0.54              |
| 52:3:884:U:H4'   | 52:3:885:G:H5''  | 1.90                     | 0.54              |
| 53:1:1268:A:H2'  | 53:1:1269:A:O4'  | 2.07                     | 0.54              |
| 1:b:224:MET:HE2  | 53:1:782:A:C6    | 2.42                     | 0.53              |
| 5:f:17:LYS:HD2   | 5:f:24:THR:HB    | 1.88                     | 0.53              |
| 17:r:81:LYS:HD2  | 53:1:973:A:H5''  | 1.90                     | 0.53              |
| 52:3:82:G:H2'    | 52:3:83:C:O4'    | 2.08                     | 0.53              |
| 52:3:1088:G:H21  | 52:3:1167:A:H61  | 1.55                     | 0.53              |
| 52:3:1524:C:H2'  | 52:3:1525:G:C8   | 2.43                     | 0.53              |
| 53:1:528:A:N1    | 53:1:2042:A:H2'  | 2.22                     | 0.53              |
| 53:1:1258:U:H2'  | 53:1:1259:G:C8   | 2.43                     | 0.53              |
| 53:1:2799:A:C2'  | 53:1:2800:A:H5'  | 2.37                     | 0.53              |
| 9:j:68:LYS:HD3   | 53:1:1022:G:N7   | 2.24                     | 0.53              |
| 52:3:505:G:H5'   | 52:3:534:U:H2'   | 1.91                     | 0.53              |
| 52:3:945:G:H2'   | 52:3:945:G:N3    | 2.23                     | 0.53              |
| 4:e:76:PHE:CE2   | 53:1:2311:A:H5'' | 2.43                     | 0.53              |
| 6:g:97:ARG:HG2   | 6:g:112:LYS:HD2  | 1.89                     | 0.53              |
| 13:n:28:LEU:HD13 | 13:n:34:ILE:HG12 | 1.89                     | 0.53              |
| 52:3:77:A:H2'    | 52:3:78:A:H8     | 1.73                     | 0.53              |
| 52:3:1259:C:H3'  | 52:3:1260:G:H5'' | 1.90                     | 0.53              |
| 53:1:2163:A:N3   | 53:1:2163:A:H2'  | 2.23                     | 0.53              |
| 37:M:91:LEU:HD12 | 37:M:92:PRO:HD2  | 1.89                     | 0.53              |
| 46:V:20:ILE:HG23 | 46:V:45:VAL:HB   | 1.90                     | 0.53              |
| 52:3:1413:A:H2   | 52:3:1487:G:H22  | 1.56                     | 0.53              |
| 17:r:35:PHE:HB2  | 17:r:59:ILE:HB   | 1.89                     | 0.53              |
| 35:K:29:ILE:HG13 | 35:K:34:GLY:HA3  | 1.89                     | 0.53              |
| 53:1:479:A:H4'   | 53:1:480:A:H5'   | 1.90                     | 0.53              |
| 53:1:2743:U:H2'  | 53:1:2744:G:O4'  | 2.09                     | 0.53              |
| 5:f:173:ALA:O    | 5:f:174:LYS:HG2  | 2.08                     | 0.53              |
| 37:M:87:ARG:HA   | 52:3:599:C:H5''  | 1.91                     | 0.53              |
| 52:3:1316:G:H2'  | 52:3:1317:C:H5'' | 1.89                     | 0.53              |
| 53:1:1060:U:H4'  | 53:1:1061:U:H5'  | 1.90                     | 0.53              |
| 53:1:2427:C:C5'  | 53:1:2429:G:H5'  | 2.37                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:l:23:ILE:HD13  | 17:r:82:HIS:CD2   | 2.43                     | 0.53              |
| 16:q:3:VAL:HG22   | 53:1:1199:U:H1'   | 1.90                     | 0.53              |
| 17:r:51:VAL:CG2   | 17:r:52:PRO:HD2   | 2.39                     | 0.53              |
| 18:s:39:THR:HG23  | 18:s:44:ALA:HB1   | 1.90                     | 0.53              |
| 41:Q:43:LYS:HG3   | 52:3:1492:A:P     | 2.49                     | 0.53              |
| 52:3:78:A:H2'     | 52:3:79:G:O4'     | 2.08                     | 0.53              |
| 53:1:362:A:H3'    | 53:1:363:G:H8     | 1.72                     | 0.53              |
| 53:1:1790:C:H2'   | 53:1:1791:A:C5    | 2.44                     | 0.53              |
| 1:b:12:ARG:HH21   | 53:1:728:G:H4'    | 1.74                     | 0.53              |
| 1:b:253:GLY:O     | 53:1:1844:C:H5'   | 2.09                     | 0.53              |
| 23:x:39:VAL:HG22  | 23:x:42:GLU:H     | 1.74                     | 0.53              |
| 33:I:57:LYS:O     | 33:I:60:VAL:HG12  | 2.09                     | 0.53              |
| 42:R:18:LEU:HD21  | 42:R:55:LEU:HD11  | 1.89                     | 0.53              |
| 49:Y:25:SER:HB3   | 52:3:1458:G:H5''  | 1.90                     | 0.53              |
| 52:3:392:C:H2'    | 52:3:393:A:H8     | 1.73                     | 0.53              |
| 53:1:942:G:H2'    | 53:1:943:A:O4'    | 2.08                     | 0.53              |
| 53:1:1438:U:H2'   | 53:1:1439:A:H8    | 1.72                     | 0.53              |
| 33:I:119:HIS:CG   | 52:3:438:U:H4'    | 2.43                     | 0.53              |
| 39:O:48:ARG:HH11  | 39:O:48:ARG:HG3   | 1.74                     | 0.53              |
| 53:1:1367:A:H2'   | 53:1:1368:G:H5'   | 1.89                     | 0.53              |
| 53:1:2048:G:H3'   | 53:1:2049:G:H5''  | 1.91                     | 0.53              |
| 7:h:13:ALA:O      | 7:h:17:GLU:HG2    | 2.09                     | 0.52              |
| 19:t:8:LEU:HD13   | 24:y:21:LEU:HG    | 1.89                     | 0.52              |
| 34:J:133:ILE:O    | 34:J:136:VAL:HG12 | 2.09                     | 0.52              |
| 53:1:278:A:H2'    | 53:1:278:A:N3     | 2.25                     | 0.52              |
| 53:1:290:U:H2'    | 53:1:291:G:H8     | 1.74                     | 0.52              |
| 53:1:554:U:H2'    | 53:1:555:G:O4'    | 2.09                     | 0.52              |
| 53:1:854:C:H2'    | 53:1:855:G:H8     | 1.73                     | 0.52              |
| 2:c:9:VAL:HB      | 2:c:26:VAL:HG23   | 1.91                     | 0.52              |
| 6:g:116:ARG:HG3   | 6:g:133:GLN:NE2   | 2.24                     | 0.52              |
| 6:g:130:VAL:HG23  | 6:g:142:VAL:HG13  | 1.90                     | 0.52              |
| 12:m:45:GLN:HE21  | 53:1:2485:G:H5''  | 1.75                     | 0.52              |
| 38:N:70:GLY:HA3   | 52:3:1371:G:O3'   | 2.07                     | 0.52              |
| 46:V:13:SER:H     | 46:V:21:VAL:HG13  | 1.73                     | 0.52              |
| 52:3:422:C:H5'    | 52:3:423:G:N3     | 2.24                     | 0.52              |
| 52:3:744:C:H2'    | 52:3:745:G:H8     | 1.75                     | 0.52              |
| 53:1:290:U:H2'    | 53:1:291:G:C8     | 2.44                     | 0.52              |
| 53:1:2215:C:H2'   | 53:1:2216:G:H8    | 1.74                     | 0.52              |
| 8:i:131:THR:O     | 8:i:135:MET:HG2   | 2.10                     | 0.52              |
| 11:l:101:ILE:HG13 | 11:l:102:GLY:N    | 2.19                     | 0.52              |
| 18:s:20:VAL:HG11  | 18:s:44:ALA:HA    | 1.91                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 20:u:50:ALA:O     | 20:u:51:LEU:HG   | 2.10                     | 0.52              |
| 43:S:86:ALA:HB1   | 43:S:91:GLU:HB2  | 1.91                     | 0.52              |
| 50:Z:50:SER:HA    | 50:Z:53:LYS:HE3  | 1.91                     | 0.52              |
| 52:3:396:C:H2'    | 52:3:397:A:H5''  | 1.90                     | 0.52              |
| 53:1:1923:U:H2'   | 53:1:1924:C:C6   | 2.44                     | 0.52              |
| 31:G:134:LEU:HD12 | 31:G:135:MET:N   | 2.24                     | 0.52              |
| 40:P:39:ASN:HB3   | 52:3:684:U:O2'   | 2.08                     | 0.52              |
| 1:b:58:LYS:NZ     | 53:1:694:U:OP2   | 2.42                     | 0.52              |
| 3:d:163:ASN:HB2   | 53:1:322:A:OP2   | 2.09                     | 0.52              |
| 9:j:123:LYS:HE2   | 53:1:7:G:H5''    | 1.90                     | 0.52              |
| 15:p:32:VAL:HG12  | 15:p:34:GLY:H    | 1.74                     | 0.52              |
| 27:C:32:LYS:HD2   | 27:C:50:GLU:HB3  | 1.90                     | 0.52              |
| 33:I:190:LEU:HD12 | 33:I:190:LEU:O   | 2.09                     | 0.52              |
| 46:V:12:VAL:HB    | 46:V:21:VAL:HG13 | 1.90                     | 0.52              |
| 15:p:20:ARG:HB3   | 15:p:21:PRO:HD2  | 1.90                     | 0.52              |
| 54:2:106:G:H2'    | 54:2:107:G:O4'   | 2.10                     | 0.52              |
| 15:p:74:GLN:HB2   | 15:p:77:SER:HB2  | 1.91                     | 0.52              |
| 17:r:6:GLN:NE2    | 17:r:37:GLU:HG2  | 2.25                     | 0.52              |
| 42:R:105:ALA:HA   | 52:3:948:C:OP1   | 2.10                     | 0.52              |
| 53:1:279:A:H2'    | 53:1:280:U:H5'   | 1.91                     | 0.52              |
| 5:f:132:LEU:HD12  | 5:f:132:LEU:O    | 2.10                     | 0.52              |
| 7:h:97:LYS:HE2    | 7:h:127:ALA:HA   | 1.91                     | 0.52              |
| 18:s:11:ARG:HD3   | 18:s:11:ARG:H    | 1.73                     | 0.52              |
| 22:w:33:ILE:HD11  | 22:w:78:ILE:HD11 | 1.91                     | 0.52              |
| 24:y:6:LEU:C      | 24:y:7:ARG:HD3   | 2.34                     | 0.52              |
| 38:N:46:VAL:HA    | 38:N:49:GLN:HG3  | 1.90                     | 0.52              |
| 42:R:22:TYR:CE1   | 52:3:1330:U:H4'  | 2.45                     | 0.52              |
| 44:T:56:LEU:O     | 44:T:59:VAL:HG12 | 2.08                     | 0.52              |
| 52:3:265:G:H2'    | 52:3:267:C:H5    | 1.75                     | 0.52              |
| 53:1:255:A:H2'    | 53:1:256:A:O4'   | 2.10                     | 0.52              |
| 9:j:97:PRO:O      | 9:j:100:VAL:HG12 | 2.10                     | 0.52              |
| 17:r:15:SER:H     | 17:r:18:GLN:NE2  | 2.08                     | 0.52              |
| 35:K:92:THR:OG1   | 35:K:93:LYS:N    | 2.39                     | 0.52              |
| 37:M:9:MET:HB2    | 37:M:32:LYS:HE2  | 1.92                     | 0.52              |
| 45:U:78:VAL:O     | 45:U:79:ASN:CB   | 2.57                     | 0.52              |
| 47:W:41:SER:HB3   | 47:W:51:GLN:HE21 | 1.74                     | 0.52              |
| 52:3:572:A:H5''   | 52:3:917:G:H4'   | 1.91                     | 0.52              |
| 52:3:744:C:H2'    | 52:3:745:G:C8    | 2.45                     | 0.52              |
| 53:1:121:G:H4'    | 53:1:149:A:H5'   | 1.92                     | 0.52              |
| 53:1:1306:C:H41   | 53:1:1606:C:H2'  | 1.75                     | 0.52              |
| 26:B:30:ASP:HB3   | 26:B:34:GLY:H    | 1.75                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:I:164:ARG:HG2  | 33:I:165:GLU:H    | 1.75                     | 0.52              |
| 45:U:68:SER:OG    | 45:U:71:VAL:HG12  | 2.10                     | 0.52              |
| 51:a:170:ILE:HG21 | 53:1:2177:C:O2    | 2.10                     | 0.52              |
| 52:3:715:A:H2'    | 52:3:716:A:C8     | 2.44                     | 0.52              |
| 52:3:1202:U:H2'   | 52:3:1203:C:H5'   | 1.92                     | 0.52              |
| 53:1:1028:A:N6    | 53:1:1125:G:H2'   | 2.25                     | 0.52              |
| 20:u:17:ASP:HB3   | 20:u:20:LYS:HD2   | 1.91                     | 0.51              |
| 21:v:30:ILE:HD11  | 21:v:38:LEU:HB3   | 1.93                     | 0.51              |
| 32:H:87:ARG:HH21  | 32:H:88:LYS:HE3   | 1.75                     | 0.51              |
| 33:I:120:LYS:HG2  | 33:I:130:ASN:OD1  | 2.09                     | 0.51              |
| 36:L:32:ASP:OD2   | 52:3:1351:U:H4'   | 2.10                     | 0.51              |
| 53:1:2799:A:H2'   | 53:1:2800:A:H5'   | 1.92                     | 0.51              |
| 17:r:74:ILE:H     | 17:r:74:ILE:HD12  | 1.76                     | 0.51              |
| 39:O:7:ARG:HD3    | 39:O:73:LEU:HD11  | 1.92                     | 0.51              |
| 49:Y:3:ILE:O      | 49:Y:4:LYS:HD3    | 2.11                     | 0.51              |
| 53:1:2710:C:H2'   | 53:1:2711:A:C8    | 2.45                     | 0.51              |
| 5:f:72:ASN:O      | 5:f:75:VAL:HG12   | 2.09                     | 0.51              |
| 7:h:80:THR:HA     | 53:1:1107:G:O2'   | 2.09                     | 0.51              |
| 17:r:59:ILE:HG22  | 17:r:98:ILE:HD11  | 1.91                     | 0.51              |
| 36:L:85:GLN:HB2   | 36:L:147:ASN:HD22 | 1.75                     | 0.51              |
| 53:1:1023:U:O2'   | 53:1:1122:G:H5'   | 2.10                     | 0.51              |
| 40:P:118:ASN:HB2  | 52:3:718:A:H5'    | 1.92                     | 0.51              |
| 48:X:15:LEU:O     | 48:X:19:GLU:HG2   | 2.11                     | 0.51              |
| 52:3:1251:A:O2'   | 52:3:1370:G:H5'   | 2.11                     | 0.51              |
| 53:1:161:A:H62    | 53:1:165:A:H61    | 1.56                     | 0.51              |
| 55:6:9:G:H5'      | 55:6:46:G:H1'     | 1.91                     | 0.51              |
| 13:n:114:GLU:HG2  | 13:n:115:LEU:N    | 2.25                     | 0.51              |
| 17:r:68:ARG:NH1   | 17:r:90:ARG:HB2   | 2.26                     | 0.51              |
| 31:G:65:LYS:HE3   | 31:G:157:PRO:HA   | 1.92                     | 0.51              |
| 40:P:34:THR:HG22  | 40:P:40:ALA:HA    | 1.93                     | 0.51              |
| 40:P:123:PRO:HG2  | 50:Z:33:ARG:HD3   | 1.92                     | 0.51              |
| 52:3:516:U:H3     | 52:3:533:A:H62    | 1.59                     | 0.51              |
| 15:p:105:LYS:HA   | 15:p:108:ARG:NH2  | 2.26                     | 0.51              |
| 45:U:5:ARG:HD2    | 52:3:376:G:H4'    | 1.91                     | 0.51              |
| 53:1:2297:A:N6    | 53:1:2319:G:H1'   | 2.26                     | 0.51              |
| 1:b:260:LYS:HA    | 1:b:263:ASP:OD2   | 2.11                     | 0.51              |
| 7:h:54:VAL:O      | 7:h:54:VAL:HG22   | 2.11                     | 0.51              |
| 10:k:13:ASN:HD22  | 52:3:339:C:P      | 2.34                     | 0.51              |
| 30:F:36:ARG:HG2   | 30:F:37:GLN:N     | 2.21                     | 0.51              |
| 48:X:18:VAL:HG11  | 48:X:43:MET:HG2   | 1.91                     | 0.51              |
| 52:3:1524:C:H2'   | 52:3:1525:G:H8    | 1.74                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:582:A:H2'   | 53:1:583:G:H8     | 1.75                     | 0.51              |
| 2:c:24:VAL:HG21  | 2:c:188:LEU:HD12  | 1.93                     | 0.51              |
| 8:i:133:ARG:NH2  | 53:1:1079:C:C4'   | 2.73                     | 0.51              |
| 29:E:22:LYS:HD3  | 29:E:46:LYS:HB2   | 1.92                     | 0.51              |
| 31:G:146:SER:OG  | 31:G:147:LEU:HD12 | 2.10                     | 0.51              |
| 40:P:51:PHE:HB3  | 40:P:55:ARG:HB3   | 1.92                     | 0.51              |
| 53:1:2122:U:H2'  | 53:1:2123:G:O4'   | 2.11                     | 0.51              |
| 25:z:5:LYS:HG3   | 25:z:57:GLU:HG3   | 1.93                     | 0.51              |
| 40:P:118:ASN:ND2 | 52:3:718:A:H5'    | 2.25                     | 0.51              |
| 53:1:171:U:H2'   | 53:1:172:A:C8     | 2.46                     | 0.51              |
| 53:1:2106:U:H2'  | 53:1:2107:G:C8    | 2.46                     | 0.51              |
| 7:h:53:ARG:HD3   | 53:1:1084:A:OP1   | 2.11                     | 0.51              |
| 17:r:24:LYS:HA   | 17:r:94:THR:OG1   | 2.11                     | 0.51              |
| 31:G:116:LEU:HB3 | 31:G:140:LEU:HD12 | 1.93                     | 0.51              |
| 41:Q:45:ASN:HD22 | 52:3:528:C:H41    | 1.58                     | 0.51              |
| 52:3:757:U:H2'   | 52:3:758:C:O4'    | 2.11                     | 0.51              |
| 53:1:1683:U:H2'  | 53:1:1684:G:C8    | 2.45                     | 0.51              |
| 53:1:2048:G:C3'  | 53:1:2049:G:H5''  | 2.40                     | 0.51              |
| 10:k:35:VAL:HG13 | 10:k:36:GLY:N     | 2.25                     | 0.50              |
| 10:k:99:ILE:HD13 | 10:k:115:ILE:HG23 | 1.93                     | 0.50              |
| 22:w:25:GLU:OE1  | 53:1:923:G:H4'    | 2.11                     | 0.50              |
| 31:G:96:LEU:O    | 31:G:99:MET:HG3   | 2.11                     | 0.50              |
| 53:1:2467:C:H2'  | 53:1:2468:A:O4'   | 2.11                     | 0.50              |
| 3:d:73:ILE:H     | 3:d:73:ILE:HD12   | 1.75                     | 0.50              |
| 52:3:352:C:H4'   | 52:3:354:G:OP1    | 2.11                     | 0.50              |
| 52:3:1412:C:H2'  | 52:3:1413:A:C8    | 2.46                     | 0.50              |
| 53:1:435:C:H2'   | 53:1:436:C:H5'    | 1.93                     | 0.50              |
| 53:1:581:C:H2'   | 53:1:582:A:C8     | 2.45                     | 0.50              |
| 53:1:2554:U:H2'  | 53:1:2555:U:C6    | 2.45                     | 0.50              |
| 8:i:52:LEU:HD21  | 8:i:73:PRO:HG2    | 1.93                     | 0.50              |
| 8:i:85:ILE:HG22  | 8:i:87:SER:H      | 1.76                     | 0.50              |
| 8:i:91:LYS:CB    | 8:i:94:LYS:HB2    | 2.40                     | 0.50              |
| 23:x:16:ASN:HB3  | 23:x:24:THR:HB    | 1.93                     | 0.50              |
| 33:I:60:VAL:O    | 33:I:63:ILE:HG12  | 2.12                     | 0.50              |
| 52:3:1005:A:H2'  | 52:3:1006:G:O4'   | 2.10                     | 0.50              |
| 53:1:1285:A:H2'  | 53:1:1286:A:H5'   | 1.92                     | 0.50              |
| 53:1:1979:U:O2'  | 53:1:1980:G:H5'   | 2.11                     | 0.50              |
| 53:1:2039:U:H2'  | 53:1:2040:G:C8    | 2.46                     | 0.50              |
| 4:e:98:PHE:HA    | 4:e:101:ARG:HE    | 1.76                     | 0.50              |
| 12:m:34:LYS:HA   | 12:m:101:VAL:HA   | 1.94                     | 0.50              |
| 18:s:57:ASN:HD21 | 53:1:494:G:H21    | 1.57                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 39:O:52:LEU:HD23 | 39:O:62:ARG:HG2   | 1.92                     | 0.50              |
| 52:3:1256:A:H1'  | 52:3:1258:G:C4    | 2.45                     | 0.50              |
| 53:1:244:A:H62   | 53:1:254:G:H21    | 1.58                     | 0.50              |
| 53:1:1053:C:C3'  | 53:1:1054:A:H5''  | 2.41                     | 0.50              |
| 1:b:143:VAL:HB   | 1:b:153:LEU:HB2   | 1.93                     | 0.50              |
| 13:n:26:GLY:HA3  | 13:n:75:ILE:HD13  | 1.93                     | 0.50              |
| 38:N:123:ARG:HB2 | 52:3:1343:G:H4'   | 1.94                     | 0.50              |
| 53:1:742:A:H2'   | 53:1:743:A:C8     | 2.47                     | 0.50              |
| 2:c:141:ARG:HH21 | 53:1:1656:C:P     | 2.34                     | 0.50              |
| 8:i:72:THR:HG21  | 8:i:112:LYS:HG2   | 1.94                     | 0.50              |
| 31:G:5:MET:HA    | 31:G:8:MET:HE3    | 1.92                     | 0.50              |
| 34:J:23:THR:HA   | 34:J:28:ARG:HA    | 1.93                     | 0.50              |
| 48:X:16:LYS:O    | 48:X:20:LYS:HG3   | 2.11                     | 0.50              |
| 49:Y:80:ALA:HA   | 49:Y:83:ASN:ND2   | 2.24                     | 0.50              |
| 53:1:729:G:H4'   | 53:1:763:G:H5'    | 1.94                     | 0.50              |
| 53:1:1720:U:H2'  | 53:1:1721:G:O4'   | 2.12                     | 0.50              |
| 53:1:1810:A:H2'  | 53:1:1811:G:O4'   | 2.12                     | 0.50              |
| 3:d:76:PRO:HA    | 3:d:82:GLY:HA2    | 1.93                     | 0.50              |
| 30:F:15:LYS:NZ   | 53:1:2753:A:H1'   | 2.26                     | 0.50              |
| 32:H:39:ARG:HA   | 32:H:54:ILE:HD11  | 1.93                     | 0.50              |
| 32:H:119:ILE:O   | 32:H:123:LEU:HG   | 2.12                     | 0.50              |
| 36:L:24:LYS:O    | 36:L:28:ILE:HG13  | 2.11                     | 0.50              |
| 37:M:91:LEU:HB3  | 37:M:116:ARG:HH11 | 1.77                     | 0.50              |
| 39:O:7:ARG:HB3   | 39:O:101:SER:OG   | 2.11                     | 0.50              |
| 44:T:23:SER:O    | 44:T:27:GLN:HG3   | 2.11                     | 0.50              |
| 48:X:12:LEU:HD12 | 48:X:13:HIS:N     | 2.26                     | 0.50              |
| 53:1:2277:G:C3'  | 53:1:2278:A:H5''  | 2.41                     | 0.50              |
| 8:i:89:SER:OG    | 8:i:135:MET:HA    | 2.12                     | 0.50              |
| 53:1:1386:C:H2'  | 53:1:1387:A:H8    | 1.77                     | 0.50              |
| 8:i:91:LYS:HA    | 8:i:91:LYS:CE     | 2.30                     | 0.50              |
| 26:B:24:VAL:HG23 | 26:B:25:THR:H     | 1.77                     | 0.50              |
| 42:R:111:PRO:HB2 | 42:R:113:LYS:HG2  | 1.94                     | 0.50              |
| 51:a:8:MET:HE2   | 53:1:2174:C:O3'   | 2.11                     | 0.50              |
| 52:3:730:G:C2'   | 52:3:731:G:H5'    | 2.42                     | 0.50              |
| 53:1:2514:U:H2'  | 53:1:2515:C:C6    | 2.47                     | 0.50              |
| 54:2:95:U:H2'    | 54:2:96:G:C8      | 2.47                     | 0.50              |
| 5:f:173:ALA:C    | 5:f:175:LYS:H     | 2.19                     | 0.49              |
| 6:g:111:ALA:O    | 6:g:115:VAL:HG23  | 2.12                     | 0.49              |
| 9:j:113:PRO:HD2  | 53:1:558:U:P      | 2.52                     | 0.49              |
| 14:o:84:GLU:OE2  | 14:o:85:LYS:HG2   | 2.11                     | 0.49              |
| 52:3:1137:C:H5'  | 52:3:1138:G:H5'   | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:1801:A:H5''  | 53:1:2203:U:H2'   | 1.93                     | 0.49              |
| 1:b:153:LEU:HD12  | 1:b:153:LEU:N     | 2.26                     | 0.49              |
| 3:d:45:ALA:HA     | 3:d:87:ALA:O      | 2.12                     | 0.49              |
| 12:m:20:LEU:HD23  | 21:v:81:PRO:HG2   | 1.93                     | 0.49              |
| 32:H:56:ILE:N     | 32:H:56:ILE:HD12  | 2.27                     | 0.49              |
| 45:U:60:TRP:HA    | 45:U:63:GLN:HB2   | 1.93                     | 0.49              |
| 52:3:291:U:H2'    | 52:3:292:G:C8     | 2.46                     | 0.49              |
| 52:3:1218:C:H2'   | 52:3:1219:A:H8    | 1.77                     | 0.49              |
| 53:1:694:U:C3'    | 53:1:695:G:H5''   | 2.42                     | 0.49              |
| 7:h:93:ALA:O      | 7:h:129:LEU:HD11  | 2.13                     | 0.49              |
| 15:p:83:ILE:HD12  | 15:p:83:ILE:N     | 2.28                     | 0.49              |
| 52:3:181:A:N6     | 52:3:194:C:H2'    | 2.28                     | 0.49              |
| 53:1:1176:U:H2'   | 53:1:1177:G:C8    | 2.47                     | 0.49              |
| 53:1:1874:C:H2'   | 53:1:1875:G:O4'   | 2.12                     | 0.49              |
| 12:m:77:PRO:O     | 12:m:80:VAL:HG12  | 2.12                     | 0.49              |
| 21:v:78:GLN:HE22  | 54:2:76:G:H1'     | 1.76                     | 0.49              |
| 53:1:799:G:H5''   | 53:1:800:A:H2'    | 1.93                     | 0.49              |
| 53:1:2475:C:C2'   | 53:1:2476:A:H5'   | 2.41                     | 0.49              |
| 4:e:39:VAL:HG13   | 4:e:40:GLY:N      | 2.28                     | 0.49              |
| 4:e:75:GLY:HA3    | 53:1:2310:C:N3    | 2.28                     | 0.49              |
| 15:p:90:ALA:HB2   | 15:p:112:ARG:HA   | 1.93                     | 0.49              |
| 32:H:122:GLN:HE21 | 32:H:125:ARG:HH22 | 1.60                     | 0.49              |
| 34:J:149:PRO:HA   | 34:J:152:VAL:HG12 | 1.94                     | 0.49              |
| 51:a:3:LYS:HD2    | 53:1:2107:G:H3'   | 1.95                     | 0.49              |
| 52:3:536:C:H2'    | 52:3:537:G:C8     | 2.48                     | 0.49              |
| 52:3:1202:U:C2'   | 52:3:1203:C:H5'   | 2.43                     | 0.49              |
| 53:1:2215:C:H2'   | 53:1:2216:G:C8    | 2.47                     | 0.49              |
| 53:1:2292:U:H2'   | 53:1:2293:G:C8    | 2.47                     | 0.49              |
| 8:i:100:ILE:HG21  | 8:i:105:LEU:HG    | 1.95                     | 0.49              |
| 14:o:15:ARG:NH2   | 54:2:8:C:H5''     | 2.27                     | 0.49              |
| 45:U:12:LYS:HG2   | 45:U:13:LYS:HG2   | 1.93                     | 0.49              |
| 52:3:56:U:H2'     | 52:3:57:G:H8      | 1.77                     | 0.49              |
| 52:3:184:G:H4'    | 52:3:224:U:H4'    | 1.92                     | 0.49              |
| 52:3:211:G:C2'    | 52:3:212:G:H5'    | 2.43                     | 0.49              |
| 52:3:1301:U:O2    | 52:3:1301:U:C2'   | 2.60                     | 0.49              |
| 53:1:2267:A:H5''  | 53:1:2268:A:H5'   | 1.95                     | 0.49              |
| 55:6:71:C:H2'     | 55:6:72:A:C8      | 2.47                     | 0.49              |
| 57:7:6:G:O2'      | 57:7:7:A:H5'      | 2.13                     | 0.49              |
| 5:f:152:ARG:NH1   | 53:1:2743:U:O2'   | 2.45                     | 0.49              |
| 13:n:92:GLY:O     | 53:1:2880:C:H1'   | 2.12                     | 0.49              |
| 17:r:78:ARG:HB3   | 17:r:83:TYR:HB3   | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:s:39:THR:HG23  | 18:s:39:THR:O     | 2.12                     | 0.49              |
| 37:M:80:PRO:HG2   | 52:3:878:A:C5'    | 2.42                     | 0.49              |
| 52:3:56:U:H2'     | 52:3:57:G:C8      | 2.47                     | 0.49              |
| 52:3:939:G:H21    | 52:3:1375:A:H2    | 1.61                     | 0.49              |
| 53:1:1438:U:H2'   | 53:1:1439:A:C8    | 2.48                     | 0.49              |
| 54:2:3:C:H3'      | 54:2:4:C:H5''     | 1.95                     | 0.49              |
| 57:7:9:A:N3       | 57:7:45:U:H2'     | 2.28                     | 0.49              |
| 1:b:140:VAL:HG12  | 1:b:191:LEU:HA    | 1.94                     | 0.49              |
| 3:d:65:THR:HG22   | 3:d:67:ARG:H      | 1.77                     | 0.49              |
| 4:e:66:ILE:H      | 4:e:66:ILE:HD12   | 1.78                     | 0.49              |
| 10:k:97:THR:O     | 10:k:118:LEU:HD13 | 2.13                     | 0.49              |
| 46:V:22:VAL:HG22  | 46:V:23:ALA:N     | 2.28                     | 0.49              |
| 52:3:350:G:H2'    | 52:3:351:G:C8     | 2.48                     | 0.49              |
| 52:3:982:U:H4'    | 52:3:983:A:O5'    | 2.12                     | 0.49              |
| 53:1:306:U:H3     | 53:1:310:A:H62    | 1.61                     | 0.49              |
| 53:1:386:G:H3'    | 53:1:387:U:H5''   | 1.94                     | 0.49              |
| 53:1:1856:U:H2'   | 53:1:1857:G:O4'   | 2.13                     | 0.49              |
| 11:l:127:VAL:HG11 | 11:l:142:ILE:HD13 | 1.94                     | 0.49              |
| 32:H:151:GLU:HG3  | 32:H:166:TRP:HB3  | 1.95                     | 0.49              |
| 41:Q:32:VAL:HB    | 41:Q:55:ARG:HB3   | 1.95                     | 0.49              |
| 41:Q:69:GLU:OE2   | 52:3:521:G:H4'    | 2.12                     | 0.49              |
| 46:V:18:LYS:HG2   | 46:V:49:ASN:HA    | 1.95                     | 0.49              |
| 50:Z:49:ALA:HA    | 52:3:723:U:O4     | 2.12                     | 0.49              |
| 53:1:534:U:H2'    | 53:1:535:G:C8     | 2.46                     | 0.49              |
| 53:1:1565:C:O2'   | 53:1:1566:A:H2'   | 2.13                     | 0.49              |
| 13:n:35:LYS:HG2   | 13:n:110:MET:HE3  | 1.95                     | 0.49              |
| 19:t:76:ARG:HH12  | 53:1:58:G:P       | 2.35                     | 0.49              |
| 26:B:10:SER:O     | 26:B:14:MET:HG3   | 2.12                     | 0.49              |
| 28:D:3:ARG:HG2    | 53:1:1613:G:H4'   | 1.94                     | 0.49              |
| 36:L:115:MET:HB2  | 52:3:1240:U:OP1   | 2.13                     | 0.49              |
| 45:U:54:LEU:HD13  | 45:U:57:ILE:HD12  | 1.95                     | 0.49              |
| 53:1:566:U:H4'    | 53:1:809:G:OP2    | 2.13                     | 0.49              |
| 53:1:2183:A:H2'   | 53:1:2184:A:C8    | 2.48                     | 0.49              |
| 53:1:2705:A:H2'   | 53:1:2706:A:O4'   | 2.13                     | 0.49              |
| 54:2:104:A:H2'    | 54:2:105:G:O4'    | 2.13                     | 0.49              |
| 26:B:24:VAL:O     | 26:B:25:THR:HG22  | 2.12                     | 0.48              |
| 33:I:3:TYR:O      | 33:I:4:LEU:HG     | 2.13                     | 0.48              |
| 33:I:145:ARG:NE   | 33:I:147:LYS:HD3  | 2.28                     | 0.48              |
| 36:L:15:PRO:HB2   | 38:N:44:ARG:NH1   | 2.28                     | 0.48              |
| 49:Y:48:LYS:O     | 49:Y:52:GLU:HG3   | 2.13                     | 0.48              |
| 51:a:62:ALA:HB2   | 51:a:162:ARG:HG2  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:3:946:A:H2'    | 52:3:947:G:C8     | 2.48                     | 0.48              |
| 52:3:1238:A:H2'   | 52:3:1239:A:H5'   | 1.95                     | 0.48              |
| 53:1:189:G:H2'    | 53:1:205:G:N2     | 2.28                     | 0.48              |
| 53:1:1111:A:H2'   | 53:1:1111:A:N3    | 2.27                     | 0.48              |
| 53:1:2200:C:H2'   | 53:1:2201:G:H8    | 1.78                     | 0.48              |
| 5:f:174:LYS:HB3   | 53:1:2529:G:H5'   | 1.95                     | 0.48              |
| 10:k:76:VAL:H     | 15:p:72:VAL:HG12  | 1.78                     | 0.48              |
| 13:n:2:ARG:HA     | 13:n:5:LYS:HD2    | 1.94                     | 0.48              |
| 38:N:121:ARG:HG3  | 52:3:1348:U:H4'   | 1.94                     | 0.48              |
| 43:S:23:ARG:HA    | 43:S:25:GLU:OE2   | 2.13                     | 0.48              |
| 51:a:172:HIS:HB3  | 53:1:2123:G:H4'   | 1.95                     | 0.48              |
| 53:1:2469:A:H2'   | 53:1:2470:G:O4'   | 2.14                     | 0.48              |
| 5:f:24:THR:HG23   | 5:f:33:THR:HG22   | 1.95                     | 0.48              |
| 6:g:78:VAL:HG21   | 6:g:103:VAL:HG12  | 1.95                     | 0.48              |
| 14:o:94:ARG:HH11  | 14:o:98:GLN:HA    | 1.78                     | 0.48              |
| 29:E:61:LEU:HD12  | 29:E:61:LEU:O     | 2.14                     | 0.48              |
| 32:H:152:VAL:HG12 | 32:H:197:VAL:HG12 | 1.95                     | 0.48              |
| 34:J:107:GLY:HA2  | 52:3:8:A:H1'      | 1.95                     | 0.48              |
| 36:L:65:LEU:O     | 36:L:69:ARG:HG3   | 2.13                     | 0.48              |
| 37:M:91:LEU:HD21  | 37:M:112:ASP:HA   | 1.95                     | 0.48              |
| 41:Q:51:VAL:HG22  | 41:Q:52:CYS:H     | 1.77                     | 0.48              |
| 47:W:31:TYR:O     | 47:W:39:VAL:HG12  | 2.13                     | 0.48              |
| 51:a:15:VAL:HG22  | 51:a:29:LEU:HD21  | 1.95                     | 0.48              |
| 52:3:543:U:H2'    | 52:3:544:G:C8     | 2.48                     | 0.48              |
| 53:1:1837:C:H2'   | 53:1:1899:A:H61   | 1.78                     | 0.48              |
| 53:1:1857:G:N2    | 53:1:1884:G:H2'   | 2.27                     | 0.48              |
| 53:1:2224:G:H4'   | 53:1:2226:C:O2    | 2.14                     | 0.48              |
| 1:b:6:LYS:HD3     | 1:b:7:PRO:HD2     | 1.95                     | 0.48              |
| 1:b:264:LYS:HE3   | 53:1:2224:G:OP1   | 2.13                     | 0.48              |
| 5:f:154:GLU:HG2   | 5:f:156:TYR:H     | 1.78                     | 0.48              |
| 8:i:20:SER:HB2    | 8:i:21:PRO:HD3    | 1.95                     | 0.48              |
| 8:i:23:VAL:CG1    | 8:i:27:LEU:HD22   | 2.44                     | 0.48              |
| 9:j:24:THR:HG23   | 9:j:27:ARG:HB2    | 1.95                     | 0.48              |
| 11:l:57:LEU:HB2   | 11:l:60:ARG:HH11  | 1.77                     | 0.48              |
| 14:o:68:LYS:HA    | 14:o:102:ARG:HG2  | 1.95                     | 0.48              |
| 25:z:29:ARG:NE    | 53:1:1183:U:H5''  | 2.27                     | 0.48              |
| 33:I:18:LEU:HD12  | 33:I:18:LEU:N     | 2.28                     | 0.48              |
| 51:a:209:ILE:HD12 | 51:a:209:ILE:N    | 2.27                     | 0.48              |
| 53:1:1417:C:H4'   | 53:1:1587:G:H21   | 1.79                     | 0.48              |
| 53:1:1437:C:H2'   | 53:1:1438:U:C6    | 2.49                     | 0.48              |
| 34:J:96:GLN:OE1   | 52:3:7:A:N6       | 2.46                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:J:97:PRO:O     | 34:J:98:ALA:C     | 2.57                     | 0.48              |
| 50:Z:66:ARG:NH2   | 52:3:1099:G:H4'   | 2.27                     | 0.48              |
| 52:3:70:U:H2'     | 52:3:94:G:O6      | 2.13                     | 0.48              |
| 52:3:166:U:H2'    | 52:3:167:A:C8     | 2.48                     | 0.48              |
| 52:3:950:U:H2'    | 52:3:951:G:C8     | 2.49                     | 0.48              |
| 53:1:1297:C:OP1   | 53:1:2710:C:H4'   | 2.14                     | 0.48              |
| 10:k:93:GLN:HG3   | 10:k:93:GLN:O     | 2.12                     | 0.48              |
| 16:q:55:GLN:HE22  | 53:1:535:G:N2     | 2.12                     | 0.48              |
| 42:R:56:ARG:O     | 42:R:59:VAL:HG12  | 2.14                     | 0.48              |
| 43:S:44:VAL:HG13  | 43:S:45:LEU:HD12  | 1.96                     | 0.48              |
| 50:Z:17:ARG:HH11  | 50:Z:20:ARG:HD2   | 1.78                     | 0.48              |
| 52:3:225:C:C3'    | 52:3:226:G:H5''   | 2.44                     | 0.48              |
| 52:3:1277:C:H2'   | 52:3:1278:G:H5''  | 1.95                     | 0.48              |
| 52:3:1356:G:H2'   | 52:3:1357:A:C8    | 2.48                     | 0.48              |
| 52:3:1502:A:H8    | 52:3:1505:G:H22   | 1.62                     | 0.48              |
| 15:p:2:ASN:OD1    | 15:p:3:ILE:HD12   | 2.13                     | 0.48              |
| 21:v:86:LEU:HD13  | 21:v:89:ILE:HD11  | 1.95                     | 0.48              |
| 38:N:114:LYS:HB2  | 38:N:117:LEU:HD12 | 1.96                     | 0.48              |
| 39:O:29:ALA:O     | 39:O:33:GLY:HA3   | 2.13                     | 0.48              |
| 39:O:88:MET:O     | 39:O:89:ARG:HD3   | 2.14                     | 0.48              |
| 40:P:63:GLN:HG3   | 40:P:98:ALA:HB2   | 1.96                     | 0.48              |
| 51:a:6:LYS:HG3    | 51:a:7:ARG:H      | 1.79                     | 0.48              |
| 53:1:639:U:H2'    | 53:1:640:C:C6     | 2.49                     | 0.48              |
| 53:1:987:C:H2'    | 53:1:988:A:O4'    | 2.13                     | 0.48              |
| 2:c:12:THR:HG22   | 2:c:13:ARG:N      | 2.29                     | 0.48              |
| 11:l:39:LYS:HD2   | 53:1:833:A:P      | 2.53                     | 0.48              |
| 23:x:7:THR:HG21   | 23:x:9:LYS:HE2    | 1.96                     | 0.48              |
| 29:E:6:VAL:HG13   | 29:E:9:ALA:HB3    | 1.96                     | 0.48              |
| 29:E:53:ASP:OD2   | 53:1:2359:C:H4'   | 2.13                     | 0.48              |
| 32:H:100:ILE:HD12 | 32:H:100:ILE:N    | 2.29                     | 0.48              |
| 50:Z:23:GLU:HB2   | 50:Z:27:VAL:HG22  | 1.96                     | 0.48              |
| 52:3:50:A:H4'     | 52:3:51:A:H5'     | 1.94                     | 0.48              |
| 52:3:779:C:H2'    | 52:3:780:A:O4'    | 2.13                     | 0.48              |
| 52:3:1401:G:H2'   | 52:3:1402:C:O4'   | 2.14                     | 0.48              |
| 53:1:482:A:H1'    | 53:1:498:G:N2     | 2.29                     | 0.48              |
| 53:1:1872:A:H2'   | 53:1:1873:G:O4'   | 2.13                     | 0.48              |
| 53:1:2853:C:H2'   | 53:1:2854:G:H8    | 1.79                     | 0.48              |
| 1:b:176:ARG:HH21  | 53:1:1820:U:H5    | 1.60                     | 0.48              |
| 1:b:239:PHE:CE2   | 1:b:243:PRO:HG3   | 2.49                     | 0.48              |
| 2:c:115:GLY:HA2   | 2:c:166:GLY:HA3   | 1.95                     | 0.48              |
| 4:e:76:PHE:HE2    | 53:1:2311:A:H5''  | 1.79                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 24:y:47:ARG:O     | 24:y:50:VAL:HG12 | 2.13                     | 0.48              |
| 41:Q:109:ARG:HH21 | 41:Q:112:ALA:HB3 | 1.79                     | 0.48              |
| 52:3:291:U:H2'    | 52:3:292:G:H8    | 1.77                     | 0.48              |
| 52:3:971:G:H1'    | 52:3:1365:G:O2'  | 2.14                     | 0.48              |
| 53:1:2313:C:H2'   | 53:1:2314:A:C8   | 2.48                     | 0.48              |
| 21:v:77:VAL:HG12  | 21:v:89:ILE:HD12 | 1.96                     | 0.48              |
| 47:W:33:THR:HG22  | 47:W:37:LYS:O    | 2.14                     | 0.48              |
| 52:3:1251:A:H2'   | 52:3:1252:A:C8   | 2.49                     | 0.48              |
| 53:1:542:C:H2'    | 53:1:543:G:H5'   | 1.96                     | 0.48              |
| 53:1:543:G:H5'    | 53:1:543:G:H8    | 1.78                     | 0.48              |
| 53:1:1386:C:H2'   | 53:1:1387:A:C8   | 2.49                     | 0.48              |
| 53:1:1528:A:H2'   | 53:1:1529:G:O4'  | 2.13                     | 0.48              |
| 53:1:1739:A:H2'   | 53:1:1740:G:O4'  | 2.14                     | 0.48              |
| 12:m:50:ARG:HH12  | 57:7:54:U:H4'    | 1.79                     | 0.47              |
| 26:B:3:GLN:HA     | 53:1:2615:U:C2   | 2.49                     | 0.47              |
| 31:G:5:MET:HE1    | 31:G:42:LEU:HB3  | 1.96                     | 0.47              |
| 33:I:103:ARG:HD2  | 33:I:167:PRO:HG2 | 1.96                     | 0.47              |
| 33:I:205:LYS:HB3  | 52:3:8:A:C6      | 2.48                     | 0.47              |
| 43:S:29:ILE:HD12  | 43:S:29:ILE:N    | 2.29                     | 0.47              |
| 53:1:818:G:O2'    | 53:1:819:A:H5''  | 2.14                     | 0.47              |
| 53:1:1078:U:H4'   | 53:1:1079:C:H5'' | 1.95                     | 0.47              |
| 53:1:1300:G:H4'   | 53:1:1301:A:H5'  | 1.96                     | 0.47              |
| 53:1:1394:U:H4'   | 53:1:1603:A:H4'  | 1.96                     | 0.47              |
| 53:1:2105:U:H2'   | 53:1:2106:U:O4'  | 2.14                     | 0.47              |
| 3:d:176:ASP:N     | 3:d:176:ASP:OD1  | 2.46                     | 0.47              |
| 4:e:63:LYS:HB3    | 54:2:42:C:H4'    | 1.96                     | 0.47              |
| 32:H:49:ALA:HA    | 32:H:74:ILE:HG21 | 1.95                     | 0.47              |
| 41:Q:4:ASN:HD22   | 46:V:35:LYS:HE3  | 1.78                     | 0.47              |
| 43:S:92:ILE:N     | 43:S:92:ILE:HD12 | 2.29                     | 0.47              |
| 52:3:543:U:H2'    | 52:3:544:G:H8    | 1.79                     | 0.47              |
| 52:3:1088:G:N2    | 52:3:1167:A:H61  | 2.13                     | 0.47              |
| 53:1:1697:G:H4'   | 53:1:1978:A:H5'' | 1.95                     | 0.47              |
| 9:j:84:ILE:HG23   | 9:j:84:ILE:O     | 2.14                     | 0.47              |
| 14:o:29:HIS:CD2   | 54:2:7:G:H5''    | 2.49                     | 0.47              |
| 19:t:58:VAL:HG13  | 19:t:85:VAL:HG22 | 1.95                     | 0.47              |
| 36:L:114:SER:O    | 36:L:118:ARG:HG3 | 2.14                     | 0.47              |
| 38:N:11:ARG:C     | 38:N:12:LYS:HG3  | 2.40                     | 0.47              |
| 49:Y:67:HIS:O     | 49:Y:69:ASN:N    | 2.45                     | 0.47              |
| 52:3:799:G:H2'    | 52:3:800:G:O4'   | 2.15                     | 0.47              |
| 52:3:1163:A:H2'   | 52:3:1164:G:C8   | 2.49                     | 0.47              |
| 53:1:91:A:H4'     | 53:1:92:U:O4'    | 2.14                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 53:1:151:C:H2'    | 53:1:152:A:C8    | 2.50                     | 0.47              |
| 53:1:616:A:H2'    | 53:1:617:G:O4'   | 2.13                     | 0.47              |
| 53:1:703:U:H2'    | 53:1:704:G:O4'   | 2.15                     | 0.47              |
| 1:b:216:ARG:NH2   | 53:1:690:G:O3'   | 2.47                     | 0.47              |
| 6:g:40:THR:OG1    | 6:g:43:ASN:ND2   | 2.48                     | 0.47              |
| 13:n:90:ARG:HH22  | 13:n:116:VAL:HB  | 1.79                     | 0.47              |
| 24:y:3:ALA:O      | 24:y:7:ARG:NH1   | 2.47                     | 0.47              |
| 30:F:25:VAL:HB    | 30:F:35:GLN:HG2  | 1.97                     | 0.47              |
| 35:K:88:MET:HE2   | 35:K:90:MET:HE2  | 1.96                     | 0.47              |
| 42:R:53:ASP:HA    | 42:R:56:ARG:HH11 | 1.79                     | 0.47              |
| 44:T:58:MET:HA    | 44:T:61:GLN:HB3  | 1.97                     | 0.47              |
| 52:3:1273:C:H2'   | 52:3:1274:A:O4'  | 2.14                     | 0.47              |
| 7:h:8:LYS:HZ2     | 7:h:11:ILE:HG13  | 1.79                     | 0.47              |
| 32:H:39:ARG:HG3   | 32:H:54:ILE:HD11 | 1.95                     | 0.47              |
| 43:S:25:GLU:HB2   | 43:S:29:ILE:HD13 | 1.96                     | 0.47              |
| 52:3:70:U:H5''    | 52:3:71:A:OP1    | 2.14                     | 0.47              |
| 52:3:79:G:O2'     | 52:3:80:A:H5'    | 2.15                     | 0.47              |
| 53:1:327:G:H2'    | 53:1:328:U:O4'   | 2.14                     | 0.47              |
| 53:1:713:G:N2     | 53:1:718:A:H62   | 2.11                     | 0.47              |
| 53:1:723:C:H2'    | 53:1:724:U:C6    | 2.50                     | 0.47              |
| 53:1:1539:U:H2'   | 53:1:1540:G:H8   | 1.79                     | 0.47              |
| 53:1:2339:C:H2'   | 53:1:2340:A:C8   | 2.50                     | 0.47              |
| 54:2:114:C:H2'    | 54:2:115:A:C8    | 2.49                     | 0.47              |
| 6:g:125:THR:HG23  | 6:g:146:VAL:O    | 2.15                     | 0.47              |
| 8:i:93:ASN:HD22   | 53:1:1077:A:H5'  | 1.78                     | 0.47              |
| 15:p:92:ARG:HD3   | 53:1:1753:G:H5'' | 1.96                     | 0.47              |
| 32:H:185:THR:HG22 | 32:H:198:LYS:HG2 | 1.96                     | 0.47              |
| 40:P:110:THR:HG22 | 50:Z:4:LYS:HG2   | 1.97                     | 0.47              |
| 42:R:24:VAL:HA    | 52:3:1329:A:H5'' | 1.96                     | 0.47              |
| 44:T:30:LEU:HD21  | 52:3:658:C:C5'   | 2.45                     | 0.47              |
| 52:3:31:G:H5'     | 52:3:306:A:C2    | 2.50                     | 0.47              |
| 52:3:67:C:H2'     | 52:3:68:G:C8     | 2.50                     | 0.47              |
| 52:3:149:A:H1'    | 52:3:1446:A:C2   | 2.49                     | 0.47              |
| 53:1:2128:G:H2'   | 53:1:2129:C:O4'  | 2.15                     | 0.47              |
| 55:5:47:U:H3'     | 55:5:48:C:C5'    | 2.45                     | 0.47              |
| 1:b:93:VAL:HG11   | 1:b:115:ILE:HD11 | 1.96                     | 0.47              |
| 2:c:4:LEU:HD22    | 2:c:32:ASN:HD22  | 1.79                     | 0.47              |
| 2:c:105:LYS:O     | 2:c:177:VAL:HG12 | 2.14                     | 0.47              |
| 2:c:155:VAL:HG21  | 53:1:2618:G:H21  | 1.80                     | 0.47              |
| 4:e:92:GLY:O      | 4:e:95:MET:HG2   | 2.15                     | 0.47              |
| 8:i:52:LEU:HD12   | 8:i:53:PRO:HD2   | 1.97                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:n:20:MET:HA   | 13:n:23:ASN:HD22  | 1.80                     | 0.47              |
| 13:n:47:VAL:O    | 13:n:50:PRO:HD2   | 2.14                     | 0.47              |
| 17:r:1:MET:HG2   | 17:r:43:ASN:ND2   | 2.30                     | 0.47              |
| 24:y:8:GLU:N     | 24:y:8:GLU:OE1    | 2.48                     | 0.47              |
| 52:3:211:G:H2'   | 52:3:212:G:H5'    | 1.96                     | 0.47              |
| 52:3:575:G:O2'   | 52:3:821:G:H5'    | 2.15                     | 0.47              |
| 53:1:151:C:H2'   | 53:1:152:A:H8     | 1.79                     | 0.47              |
| 53:1:176:A:H3'   | 53:1:177:G:N2     | 2.30                     | 0.47              |
| 53:1:1161:C:H2'  | 53:1:1162:G:C8    | 2.50                     | 0.47              |
| 53:1:1909:C:H2'  | 53:1:1910:G:H8    | 1.80                     | 0.47              |
| 53:1:2494:G:H2'  | 53:1:2495:G:H8    | 1.78                     | 0.47              |
| 8:i:90:GLY:O     | 8:i:91:LYS:HE3    | 2.15                     | 0.47              |
| 28:D:26:ASN:CG   | 53:1:682:G:H5'    | 2.40                     | 0.47              |
| 34:J:55:VAL:HG13 | 34:J:56:PRO:HD3   | 1.97                     | 0.47              |
| 40:P:22:ILE:HG23 | 40:P:85:VAL:HA    | 1.96                     | 0.47              |
| 53:1:873:C:H2'   | 53:1:874:G:C8     | 2.50                     | 0.47              |
| 53:1:1360:G:H22  | 53:1:2214:C:H42   | 1.62                     | 0.47              |
| 53:1:2055:C:H2'  | 53:1:2504:U:H5'   | 1.96                     | 0.47              |
| 55:6:16:C:O2'    | 55:6:17:C:H5'     | 2.15                     | 0.47              |
| 3:d:84:THR:HG21  | 53:1:672:C:H5''   | 1.97                     | 0.47              |
| 4:e:72:SER:OG    | 55:5:56:C:H4'     | 2.14                     | 0.47              |
| 14:o:16:ARG:HD3  | 14:o:19:GLN:NE2   | 2.30                     | 0.47              |
| 30:F:16:ILE:N    | 30:F:16:ILE:HD12  | 2.30                     | 0.47              |
| 38:N:57:VAL:HG23 | 38:N:58:GLU:OE1   | 2.15                     | 0.47              |
| 41:Q:120:ARG:NH1 | 52:3:500:G:H5'    | 2.30                     | 0.47              |
| 42:R:90:HIS:HA   | 42:R:108:ARG:NH2  | 2.30                     | 0.47              |
| 53:1:305:C:H2'   | 53:1:306:U:C6     | 2.49                     | 0.47              |
| 54:2:2:G:H2'     | 54:2:3:C:C6       | 2.50                     | 0.47              |
| 54:2:66:A:H4'    | 54:2:67:G:C8      | 2.50                     | 0.47              |
| 1:b:30:ALA:HB3   | 1:b:31:PRO:HD3    | 1.97                     | 0.47              |
| 18:s:41:LYS:CD   | 53:1:2009:A:H5''  | 2.44                     | 0.47              |
| 18:s:88:ARG:HH12 | 53:1:2013:A:H2    | 1.63                     | 0.47              |
| 21:v:60:VAL:HG22 | 21:v:73:LYS:HD3   | 1.97                     | 0.47              |
| 41:Q:109:ARG:HB3 | 41:Q:118:VAL:HG21 | 1.97                     | 0.47              |
| 44:T:85:GLY:C    | 44:T:86:LEU:HD12  | 2.40                     | 0.47              |
| 50:Z:23:GLU:C    | 50:Z:25:ALA:H     | 2.23                     | 0.47              |
| 52:3:1001:C:H2'  | 52:3:1002:G:C8    | 2.50                     | 0.47              |
| 53:1:861:A:H2'   | 53:1:862:G:O4'    | 2.15                     | 0.47              |
| 53:1:1758:U:C5   | 53:1:2696:U:H5'   | 2.49                     | 0.47              |
| 53:1:2282:G:H4'  | 53:1:2389:G:O2'   | 2.15                     | 0.47              |
| 11:l:74:THR:HG22 | 11:l:107:PHE:HB2  | 1.96                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:p:113:LEU:O   | 15:p:113:LEU:HD12 | 2.14                     | 0.46              |
| 34:J:19:ARG:HB3  | 34:J:32:PHE:CE1   | 2.50                     | 0.46              |
| 50:Z:23:GLU:O    | 50:Z:25:ALA:N     | 2.46                     | 0.46              |
| 52:3:946:A:H2'   | 52:3:947:G:H8     | 1.80                     | 0.46              |
| 52:3:978:A:H4'   | 52:3:1322:C:N3    | 2.30                     | 0.46              |
| 52:3:1404:C:H2'  | 52:3:1405:G:C8    | 2.51                     | 0.46              |
| 53:1:69:C:O2'    | 53:1:70:G:H5'     | 2.14                     | 0.46              |
| 53:1:191:A:H2'   | 53:1:192:C:C6     | 2.50                     | 0.46              |
| 53:1:971:G:H2'   | 53:1:972:A:O4'    | 2.15                     | 0.46              |
| 53:1:1344:U:H3'  | 53:1:1345:C:H5'   | 1.96                     | 0.46              |
| 53:1:2093:G:N7   | 53:1:2225:A:H2'   | 2.29                     | 0.46              |
| 53:1:2853:C:H2'  | 53:1:2854:G:C8    | 2.50                     | 0.46              |
| 33:I:50:TYR:CD2  | 52:3:508:U:H4'    | 2.51                     | 0.46              |
| 36:L:72:VAL:HG12 | 36:L:89:GLU:HA    | 1.97                     | 0.46              |
| 52:3:1125:U:H2'  | 52:3:1126:U:H2'   | 1.97                     | 0.46              |
| 53:1:546:U:H2'   | 53:1:547:A:H4'    | 1.97                     | 0.46              |
| 53:1:2093:G:H21  | 53:1:2198:A:N6    | 2.13                     | 0.46              |
| 54:2:5:U:H2'     | 54:2:6:G:H8       | 1.81                     | 0.46              |
| 2:c:56:LYS:NZ    | 53:1:2830:C:OP1   | 2.48                     | 0.46              |
| 6:g:132:PHE:HB2  | 6:g:140:ALA:HB3   | 1.96                     | 0.46              |
| 15:p:52:ARG:NH2  | 53:1:2720:U:H5''  | 2.31                     | 0.46              |
| 15:p:108:ARG:HE  | 52:3:1463:U:P     | 2.38                     | 0.46              |
| 31:G:162:VAL:HB  | 31:G:184:ALA:CB   | 2.45                     | 0.46              |
| 43:S:33:VAL:O    | 43:S:33:VAL:HG22  | 2.15                     | 0.46              |
| 44:T:25:GLU:HG2  | 44:T:80:LEU:HD13  | 1.97                     | 0.46              |
| 53:1:941:A:H2'   | 53:1:942:G:O4'    | 2.15                     | 0.46              |
| 53:1:2221:G:O2'  | 53:1:2222:C:H5'   | 2.15                     | 0.46              |
| 54:2:63:C:H2'    | 54:2:64:G:H8      | 1.79                     | 0.46              |
| 3:d:40:ARG:HD2   | 53:1:443:A:C6     | 2.50                     | 0.46              |
| 19:t:54:GLU:HB3  | 19:t:88:LYS:HD2   | 1.98                     | 0.46              |
| 20:u:31:GLY:O    | 20:u:66:VAL:HG23  | 2.16                     | 0.46              |
| 21:v:70:ILE:H    | 21:v:70:ILE:HD12  | 1.81                     | 0.46              |
| 40:P:58:THR:HG23 | 40:P:61:ALA:H     | 1.80                     | 0.46              |
| 42:R:85:TYR:CE2  | 52:3:1321:U:H5''  | 2.51                     | 0.46              |
| 52:3:5:U:H4'     | 52:3:6:G:C8       | 2.51                     | 0.46              |
| 52:3:323:U:H2'   | 52:3:324:G:O4'    | 2.15                     | 0.46              |
| 52:3:629:A:H2'   | 52:3:630:A:O4'    | 2.15                     | 0.46              |
| 53:1:1983:G:H4'  | 53:1:2606:C:H4'   | 1.96                     | 0.46              |
| 53:1:2051:A:H2'  | 53:1:2578:G:OP1   | 2.15                     | 0.46              |
| 54:2:63:C:H2'    | 54:2:64:G:C8      | 2.51                     | 0.46              |
| 1:b:200:MET:HG3  | 53:1:1820:U:C2    | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:f:174:LYS:HE2   | 53:1:2531:A:OP1   | 2.16                     | 0.46              |
| 32:H:69:THR:OG1   | 32:H:70:ALA:N     | 2.48                     | 0.46              |
| 34:J:87:VAL:HA    | 34:J:91:SER:O     | 2.15                     | 0.46              |
| 37:M:104:SER:HB2  | 37:M:125:ILE:HD11 | 1.97                     | 0.46              |
| 43:S:100:TRP:HZ2  | 52:3:1368:A:H5''  | 1.79                     | 0.46              |
| 46:V:22:VAL:HG22  | 46:V:23:ALA:H     | 1.81                     | 0.46              |
| 52:3:206:C:H2'    | 52:3:207:C:O4'    | 2.15                     | 0.46              |
| 53:1:741:U:H2'    | 53:1:742:A:C8     | 2.51                     | 0.46              |
| 53:1:826:U:H5''   | 53:1:2429:G:P     | 2.55                     | 0.46              |
| 53:1:1079:C:H2'   | 53:1:1080:A:C8    | 2.51                     | 0.46              |
| 53:1:1421:G:H1'   | 53:1:1494:A:H61   | 1.81                     | 0.46              |
| 53:1:2345:G:N3    | 53:1:2381:A:H2'   | 2.30                     | 0.46              |
| 53:1:2861:U:H2'   | 53:1:2862:G:C8    | 2.50                     | 0.46              |
| 54:2:19:C:H2'     | 54:2:20:G:C8      | 2.50                     | 0.46              |
| 26:B:28:SER:HB2   | 53:1:2885:G:O6    | 2.16                     | 0.46              |
| 32:H:154:GLY:HA2  | 52:3:1057:G:H5'   | 1.98                     | 0.46              |
| 33:I:49:ASP:O     | 33:I:52:VAL:HG12  | 2.14                     | 0.46              |
| 36:L:87:PRO:HD3   | 36:L:147:ASN:O    | 2.16                     | 0.46              |
| 39:O:44:THR:HG23  | 39:O:69:THR:C     | 2.40                     | 0.46              |
| 40:P:71:ASP:O     | 40:P:72:ALA:HB3   | 2.15                     | 0.46              |
| 41:Q:50:LYS:HD3   | 41:Q:71:HIS:CE1   | 2.51                     | 0.46              |
| 42:R:3:ILE:HG12   | 42:R:7:ASN:HD22   | 1.81                     | 0.46              |
| 51:a:6:LYS:HA     | 51:a:9:ARG:HH21   | 1.81                     | 0.46              |
| 52:3:664:G:H22    | 52:3:741:G:H1     | 1.62                     | 0.46              |
| 52:3:1139:G:H5''  | 52:3:1140:C:H5    | 1.79                     | 0.46              |
| 53:1:239:C:H2'    | 53:1:240:C:O4'    | 2.15                     | 0.46              |
| 53:1:794:A:H2'    | 53:1:795:C:C6     | 2.51                     | 0.46              |
| 53:1:1161:C:H2'   | 53:1:1162:G:H8    | 1.81                     | 0.46              |
| 53:1:1298:C:H2'   | 53:1:1299:G:O4'   | 2.15                     | 0.46              |
| 53:1:2281:A:O2'   | 53:1:2282:G:H5'   | 2.16                     | 0.46              |
| 53:1:2834:G:O2'   | 53:1:2835:A:H5'   | 2.16                     | 0.46              |
| 1:b:52:HIS:HA     | 1:b:216:ARG:HB3   | 1.97                     | 0.46              |
| 13:n:33:ILE:O     | 13:n:33:ILE:HG13  | 2.16                     | 0.46              |
| 18:s:37:THR:HG22  | 18:s:48:LYS:HE3   | 1.96                     | 0.46              |
| 33:I:145:ARG:CZ   | 33:I:147:LYS:HD3  | 2.46                     | 0.46              |
| 40:P:112:VAL:HG22 | 40:P:112:VAL:O    | 2.16                     | 0.46              |
| 40:P:125:LYS:O    | 40:P:126:ARG:HB2  | 2.15                     | 0.46              |
| 53:1:2220:U:H2'   | 53:1:2221:G:H8    | 1.80                     | 0.46              |
| 53:1:2364:C:H2'   | 53:1:2365:G:O4'   | 2.16                     | 0.46              |
| 53:1:2698:U:H2'   | 53:1:2699:C:C6    | 2.51                     | 0.46              |
| 26:B:15:ARG:NH1   | 53:1:1264:A:OP1   | 2.49                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:F:36:ARG:CG   | 30:F:37:GLN:H    | 2.13                     | 0.46              |
| 31:G:113:LEU:O   | 31:G:117:GLU:HG3 | 2.16                     | 0.46              |
| 38:N:11:ARG:O    | 38:N:12:LYS:HG3  | 2.16                     | 0.46              |
| 41:Q:51:VAL:HG22 | 41:Q:52:CYS:N    | 2.31                     | 0.46              |
| 43:S:3:GLN:HG3   | 43:S:6:LYS:HZ3   | 1.81                     | 0.46              |
| 45:U:1:MET:HB2   | 52:3:135:C:N3    | 2.30                     | 0.46              |
| 52:3:802:A:H2'   | 52:3:803:G:O4'   | 2.16                     | 0.46              |
| 52:3:1071:C:H2'  | 52:3:1072:G:H8   | 1.80                     | 0.46              |
| 52:3:1287:A:H2   | 52:3:1353:G:H1'  | 1.80                     | 0.46              |
| 53:1:320:A:H2    | 53:1:323:C:H41   | 1.62                     | 0.46              |
| 53:1:492:A:H2'   | 53:1:493:G:O4'   | 2.16                     | 0.46              |
| 53:1:562:U:H2'   | 53:1:572:A:O4'   | 2.16                     | 0.46              |
| 2:c:202:ILE:HD12 | 2:c:202:ILE:N    | 2.30                     | 0.46              |
| 28:D:34:ARG:HH12 | 53:1:466:A:P     | 2.38                     | 0.46              |
| 29:E:5:THR:HG22  | 29:E:62:PRO:HD2  | 1.97                     | 0.46              |
| 30:F:32:LYS:HE2  | 53:1:2478:A:OP1  | 2.16                     | 0.46              |
| 32:H:38:VAL:O    | 32:H:42:LEU:HD23 | 2.15                     | 0.46              |
| 52:3:411:A:C4    | 52:3:413:G:H1'   | 2.50                     | 0.46              |
| 52:3:663:A:H5'   | 52:3:836:G:OP1   | 2.16                     | 0.46              |
| 52:3:1115:U:H2'  | 52:3:1116:U:C6   | 2.51                     | 0.46              |
| 52:3:1298:U:H4'  | 52:3:1299:A:O4'  | 2.16                     | 0.46              |
| 52:3:1527:U:O2'  | 52:3:1528:U:H5'  | 2.15                     | 0.46              |
| 53:1:395:U:H2'   | 53:1:396:G:C8    | 2.51                     | 0.46              |
| 53:1:1077:A:C2'  | 53:1:1078:U:H5'  | 2.45                     | 0.46              |
| 12:m:13:HIS:CG   | 53:1:954:G:H5''  | 2.51                     | 0.46              |
| 16:q:111:LYS:HB2 | 17:r:48:LYS:HZ2  | 1.79                     | 0.46              |
| 32:H:198:LYS:HD2 | 52:3:1058:G:OP1  | 2.16                     | 0.46              |
| 48:X:28:LYS:O    | 48:X:30:LEU:HD12 | 2.16                     | 0.46              |
| 48:X:44:ILE:HD13 | 48:X:63:ASP:HA   | 1.98                     | 0.46              |
| 49:Y:77:ASN:O    | 49:Y:81:GLN:HG2  | 2.16                     | 0.46              |
| 52:3:20:U:H2'    | 52:3:21:G:O4'    | 2.15                     | 0.46              |
| 52:3:559:A:H4'   | 52:3:560:A:H3'   | 1.98                     | 0.46              |
| 52:3:1464:U:H2'  | 52:3:1465:A:H8   | 1.81                     | 0.46              |
| 53:1:277:G:H1'   | 53:1:361:G:O6    | 2.16                     | 0.46              |
| 53:1:374:A:H2'   | 53:1:375:G:O4'   | 2.16                     | 0.46              |
| 53:1:2257:U:O2'  | 53:1:2258:C:H5'  | 2.16                     | 0.46              |
| 4:e:34:THR:OG1   | 4:e:154:THR:HB   | 2.15                     | 0.45              |
| 7:h:50:VAL:HG13  | 53:1:1083:U:OP2  | 2.17                     | 0.45              |
| 13:n:69:ARG:C    | 13:n:71:ARG:H    | 2.24                     | 0.45              |
| 26:B:27:LEU:HD23 | 26:B:36:LYS:HB3  | 1.97                     | 0.45              |
| 39:O:57:VAL:O    | 39:O:58:ASN:CB   | 2.63                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:1:1045:C:H5'  | 53:1:1046:A:C5'  | 2.46                     | 0.45              |
| 53:1:2141:G:H22  | 53:1:2151:U:H1'  | 1.80                     | 0.45              |
| 2:c:135:GLY:HA2  | 53:1:743:A:OP1   | 2.16                     | 0.45              |
| 10:k:6:THR:HG23  | 53:1:1666:G:H4'  | 1.97                     | 0.45              |
| 16:q:87:VAL:HG12 | 16:q:89:ILE:HG13 | 1.99                     | 0.45              |
| 20:u:3:LYS:O     | 20:u:93:ARG:NH2  | 2.49                     | 0.45              |
| 28:D:34:ARG:NE   | 28:D:39:ARG:HD2  | 2.32                     | 0.45              |
| 39:O:37:ARG:HG3  | 52:3:1124:G:H5'' | 1.98                     | 0.45              |
| 48:X:18:VAL:O    | 48:X:22:VAL:HG23 | 2.17                     | 0.45              |
| 51:a:205:LYS:HG3 | 53:1:1861:G:H5'  | 1.97                     | 0.45              |
| 52:3:909:A:H2'   | 52:3:910:C:O4'   | 2.16                     | 0.45              |
| 53:1:457:A:N1    | 53:1:470:A:H5''  | 2.31                     | 0.45              |
| 53:1:2818:U:H2'  | 53:1:2819:G:C8   | 2.50                     | 0.45              |
| 54:2:88:C:O2'    | 54:2:89:U:O5'    | 2.29                     | 0.45              |
| 2:c:56:LYS:HG3   | 2:c:58:ASN:OD1   | 2.16                     | 0.45              |
| 3:d:142:ALA:O    | 3:d:143:LEU:HD22 | 2.16                     | 0.45              |
| 5:f:173:ALA:O    | 5:f:175:LYS:N    | 2.48                     | 0.45              |
| 7:h:53:ARG:HD2   | 7:h:55:VAL:HG13  | 1.97                     | 0.45              |
| 21:v:30:ILE:HG22 | 21:v:91:PHE:HB2  | 1.98                     | 0.45              |
| 40:P:91:GLY:C    | 40:P:93:GLU:H    | 2.25                     | 0.45              |
| 52:3:194:C:O2'   | 52:3:195:A:H5'   | 2.17                     | 0.45              |
| 52:3:346:G:C2'   | 52:3:347:G:H5'   | 2.47                     | 0.45              |
| 53:1:340:A:H2'   | 53:1:341:C:O4'   | 2.16                     | 0.45              |
| 53:1:1138:G:H2'  | 53:1:1139:G:O4'  | 2.16                     | 0.45              |
| 57:7:49:C:H6     | 57:7:49:C:H5'    | 1.81                     | 0.45              |
| 20:u:85:ARG:CD   | 20:u:87:GLU:HG3  | 2.46                     | 0.45              |
| 50:Z:23:GLU:O    | 50:Z:24:LYS:HG2  | 2.16                     | 0.45              |
| 53:1:687:C:H2'   | 53:1:688:U:O4'   | 2.16                     | 0.45              |
| 1:b:68:ARG:O     | 1:b:188:ARG:NH1  | 2.50                     | 0.45              |
| 6:g:112:LYS:HZ1  | 53:1:2221:G:P    | 2.39                     | 0.45              |
| 10:k:23:LYS:HE2  | 10:k:23:LYS:HB2  | 1.78                     | 0.45              |
| 31:G:166:ASP:HB2 | 31:G:190:SER:HB3 | 1.98                     | 0.45              |
| 32:H:4:VAL:HG22  | 32:H:5:HIS:N     | 2.30                     | 0.45              |
| 37:M:28:SER:OG   | 37:M:29:SER:N    | 2.48                     | 0.45              |
| 48:X:2:ARG:HD3   | 48:X:2:ARG:N     | 2.32                     | 0.45              |
| 52:3:494:G:H2'   | 52:3:496:A:H8    | 1.80                     | 0.45              |
| 52:3:1114:C:H2'  | 52:3:1115:U:O4'  | 2.16                     | 0.45              |
| 53:1:481:G:H1'   | 53:1:506:G:N2    | 2.31                     | 0.45              |
| 53:1:1507:C:H2'  | 53:1:1508:A:O4'  | 2.15                     | 0.45              |
| 53:1:2004:G:H2'  | 53:1:2005:A:O4'  | 2.17                     | 0.45              |
| 53:1:2339:C:H2'  | 53:1:2340:A:H8   | 1.82                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:2421:G:H2'   | 55:6:76:A:N6      | 2.32                     | 0.45              |
| 53:1:2699:C:H2'   | 53:1:2700:A:C8    | 2.51                     | 0.45              |
| 8:i:93:ASN:ND2    | 53:1:1076:C:O3'   | 2.50                     | 0.45              |
| 33:I:112:GLU:O    | 33:I:116:LEU:HG   | 2.16                     | 0.45              |
| 36:L:16:LYS:HD2   | 36:L:17:PHE:CD1   | 2.52                     | 0.45              |
| 38:N:83:THR:HG21  | 38:N:102:PHE:HB3  | 1.97                     | 0.45              |
| 40:P:118:ASN:HD22 | 52:3:718:A:C5'    | 2.29                     | 0.45              |
| 45:U:20:VAL:HG22  | 45:U:21:VAL:N     | 2.32                     | 0.45              |
| 51:a:163:TYR:HB3  | 51:a:173:THR:HG22 | 1.99                     | 0.45              |
| 52:3:513:C:H2'    | 52:3:514:C:C6     | 2.50                     | 0.45              |
| 52:3:555:U:H2'    | 52:3:556:C:C6     | 2.50                     | 0.45              |
| 52:3:855:U:H2'    | 52:3:856:C:C6     | 2.51                     | 0.45              |
| 53:1:457:A:H61    | 53:1:470:A:H5''   | 1.82                     | 0.45              |
| 55:6:6:G:O2'      | 55:6:7:G:H5'      | 2.16                     | 0.45              |
| 6:g:63:ALA:HA     | 6:g:66:ASN:ND2    | 2.30                     | 0.45              |
| 8:i:74:PRO:HB2    | 8:i:77:VAL:HG22   | 1.98                     | 0.45              |
| 8:i:101:SER:HB3   | 8:i:104:GLN:HG3   | 1.99                     | 0.45              |
| 10:k:23:LYS:NZ    | 53:1:2548:U:O2    | 2.47                     | 0.45              |
| 13:n:3:HIS:CD2    | 53:1:2820:A:H4'   | 2.52                     | 0.45              |
| 14:o:31:THR:HG23  | 14:o:34:HIS:O     | 2.17                     | 0.45              |
| 15:p:105:LYS:HD3  | 15:p:108:ARG:NH2  | 2.32                     | 0.45              |
| 33:I:7:LYS:HG3    | 33:I:21:LYS:HD3   | 1.98                     | 0.45              |
| 39:O:59:LYS:HE2   | 39:O:62:ARG:HH21  | 1.81                     | 0.45              |
| 43:S:30:ILE:HG22  | 43:S:43:ALA:HB2   | 1.99                     | 0.45              |
| 46:V:13:SER:H     | 46:V:21:VAL:CG1   | 2.30                     | 0.45              |
| 52:3:225:C:C2'    | 52:3:226:G:H5''   | 2.47                     | 0.45              |
| 52:3:1170:A:H2'   | 52:3:1171:A:O4'   | 2.16                     | 0.45              |
| 53:1:582:A:H2'    | 53:1:583:G:C8     | 2.52                     | 0.45              |
| 53:1:2537:U:H2'   | 53:1:2538:C:C6    | 2.50                     | 0.45              |
| 53:1:2818:U:H2'   | 53:1:2819:G:H8    | 1.82                     | 0.45              |
| 5:f:86:LEU:HB2    | 5:f:130:ILE:HB    | 1.99                     | 0.45              |
| 15:p:17:PRO:HG3   | 15:p:83:ILE:HB    | 1.99                     | 0.45              |
| 24:y:24:GLU:O     | 24:y:28:LEU:HD23  | 2.17                     | 0.45              |
| 25:z:40:THR:O     | 25:z:43:ILE:HG22  | 2.16                     | 0.45              |
| 41:Q:48:LEU:HB2   | 52:3:520:A:OP1    | 2.16                     | 0.45              |
| 45:U:33:ILE:H     | 45:U:33:ILE:HD12  | 1.82                     | 0.45              |
| 50:Z:57:LYS:O     | 50:Z:61:ARG:HG3   | 2.17                     | 0.45              |
| 52:3:1195:C:H5''  | 52:3:1196:A:OP2   | 2.16                     | 0.45              |
| 52:3:1201:A:C1'   | 52:3:1202:U:OP2   | 2.62                     | 0.45              |
| 53:1:1103:A:H2'   | 53:1:1103:A:N3    | 2.32                     | 0.45              |
| 53:1:2737:G:H2'   | 53:1:2738:A:C8    | 2.52                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:729:G:H4'   | 53:1:763:G:C5'    | 2.47                     | 0.45              |
| 53:1:1020:A:C1'  | 53:1:1021:A:OP2   | 2.61                     | 0.45              |
| 53:1:1775:U:H2'  | 53:1:1776:G:O4'   | 2.16                     | 0.45              |
| 53:1:2144:G:H1'  | 53:1:2147:A:H61   | 1.81                     | 0.45              |
| 53:1:2629:U:O2'  | 53:1:2630:G:H5''  | 2.16                     | 0.45              |
| 54:2:95:U:H2'    | 54:2:96:G:H8      | 1.80                     | 0.45              |
| 4:e:29:ARG:HG2   | 4:e:29:ARG:HH11   | 1.82                     | 0.45              |
| 13:n:73:ASN:HA   | 13:n:76:VAL:HG12  | 1.97                     | 0.45              |
| 16:q:25:GLY:O    | 16:q:29:ARG:NH1   | 2.50                     | 0.45              |
| 16:q:116:LEU:O   | 16:q:116:LEU:HD23 | 2.16                     | 0.45              |
| 31:G:40:ILE:H    | 31:G:40:ILE:HD12  | 1.82                     | 0.45              |
| 48:X:30:LEU:HD12 | 48:X:30:LEU:H     | 1.82                     | 0.45              |
| 48:X:77:ARG:HH12 | 52:3:1322:C:P     | 2.39                     | 0.45              |
| 52:3:161:A:H2    | 52:3:347:G:H21    | 1.65                     | 0.45              |
| 52:3:1160:G:H1   | 52:3:1176:A:H61   | 1.65                     | 0.45              |
| 53:1:310:A:H2'   | 53:1:311:A:H5''   | 1.99                     | 0.45              |
| 53:1:532:A:H2'   | 53:1:532:A:N3     | 2.32                     | 0.45              |
| 54:2:108:A:H5'   | 54:2:109:A:O5'    | 2.17                     | 0.45              |
| 3:d:23:PHE:HE2   | 3:d:25:GLU:HG3    | 1.83                     | 0.44              |
| 7:h:67:THR:HB    | 7:h:68:PRO:HD3    | 1.99                     | 0.44              |
| 10:k:34:GLY:N    | 10:k:37:ASP:OD2   | 2.50                     | 0.44              |
| 19:t:4:GLU:HA    | 19:t:7:LEU:HB2    | 1.98                     | 0.44              |
| 20:u:5:ARG:HG3   | 20:u:93:ARG:NH2   | 2.32                     | 0.44              |
| 20:u:42:LYS:HD2  | 53:1:499:U:H5''   | 1.97                     | 0.44              |
| 21:v:42:LEU:H    | 21:v:42:LEU:HD23  | 1.81                     | 0.44              |
| 35:K:26:THR:O    | 35:K:29:ILE:HG22  | 2.17                     | 0.44              |
| 37:M:74:ILE:HG23 | 37:M:74:ILE:O     | 2.17                     | 0.44              |
| 41:Q:50:LYS:HD3  | 41:Q:71:HIS:HE1   | 1.82                     | 0.44              |
| 43:S:27:LYS:HD3  | 43:S:47:LEU:HD11  | 1.98                     | 0.44              |
| 52:3:1163:A:H2'  | 52:3:1164:G:H8    | 1.80                     | 0.44              |
| 53:1:1045:C:P    | 53:1:1047:G:H5'   | 2.57                     | 0.44              |
| 53:1:2475:C:H42  | 53:1:2529:G:H22   | 1.65                     | 0.44              |
| 53:1:2636:C:H2'  | 53:1:2637:U:C6    | 2.51                     | 0.44              |
| 53:1:2813:A:H2'  | 53:1:2814:A:O4'   | 2.17                     | 0.44              |
| 1:b:97:ASP:OD2   | 53:1:1491:G:H5'   | 2.18                     | 0.44              |
| 5:f:32:LEU:HD12  | 5:f:78:VAL:HG13   | 1.99                     | 0.44              |
| 9:j:100:VAL:HG13 | 9:j:101:ILE:N     | 2.33                     | 0.44              |
| 12:m:38:ARG:HG3  | 12:m:98:PRO:HD3   | 1.98                     | 0.44              |
| 19:t:68:LYS:HE3  | 53:1:1336:A:OP2   | 2.17                     | 0.44              |
| 29:E:51:LYS:HA   | 29:E:54:LEU:HD22  | 1.99                     | 0.44              |
| 31:G:69:VAL:HG22 | 31:G:161:PHE:O    | 2.17                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:G:112:ARG:O   | 31:G:116:LEU:HD13 | 2.16                     | 0.44              |
| 51:a:30:LEU:HD22 | 51:a:216:THR:HG23 | 1.98                     | 0.44              |
| 52:3:58:C:O2'    | 52:3:59:A:H5'     | 2.17                     | 0.44              |
| 52:3:1071:C:H2'  | 52:3:1072:G:C8    | 2.52                     | 0.44              |
| 53:1:818:G:C2'   | 53:1:819:A:H5''   | 2.47                     | 0.44              |
| 53:1:1906:G:C3'  | 53:1:1907:G:H5''  | 2.47                     | 0.44              |
| 53:1:2586:U:H2'  | 53:1:2587:A:C8    | 2.52                     | 0.44              |
| 55:6:48:C:O2'    | 55:6:59:A:H1'     | 2.16                     | 0.44              |
| 2:c:15:PHE:HE2   | 15:p:54:LEU:HD21  | 1.82                     | 0.44              |
| 8:i:94:LYS:NZ    | 53:1:1076:C:H4'   | 2.31                     | 0.44              |
| 9:j:8:PRO:HG3    | 9:j:48:VAL:HG13   | 1.98                     | 0.44              |
| 16:q:20:ALA:HA   | 16:q:23:TYR:CE2   | 2.52                     | 0.44              |
| 26:B:8:THR:OG1   | 26:B:9:ARG:N      | 2.50                     | 0.44              |
| 37:M:50:VAL:HG22 | 37:M:50:VAL:O     | 2.17                     | 0.44              |
| 52:3:405:U:C3'   | 52:3:406:G:H5'    | 2.46                     | 0.44              |
| 53:1:69:C:H2'    | 53:1:70:G:C8      | 2.53                     | 0.44              |
| 53:1:281:C:N4    | 53:1:359:G:H1     | 2.12                     | 0.44              |
| 53:1:694:U:H3'   | 53:1:695:G:H5''   | 1.98                     | 0.44              |
| 53:1:1991:U:H2'  | 53:1:1992:G:C5'   | 2.48                     | 0.44              |
| 53:1:2248:C:C2'  | 53:1:2249:U:H5'   | 2.47                     | 0.44              |
| 53:1:2412:A:H2'  | 53:1:2413:G:O4'   | 2.17                     | 0.44              |
| 53:1:2529:G:H5'' | 53:1:2530:A:H5''  | 1.99                     | 0.44              |
| 3:d:68:ALA:HA    | 53:1:1255:U:C6    | 2.53                     | 0.44              |
| 16:q:47:ARG:NH2  | 16:q:51:GLN:HE22  | 2.12                     | 0.44              |
| 17:r:52:PRO:O    | 17:r:53:PHE:HB2   | 2.17                     | 0.44              |
| 23:x:18:SER:OG   | 23:x:19:HIS:N     | 2.50                     | 0.44              |
| 34:J:121:ASN:OD1 | 34:J:122:VAL:HG13 | 2.16                     | 0.44              |
| 34:J:159:SER:O   | 34:J:162:GLU:HG3  | 2.18                     | 0.44              |
| 38:N:7:GLY:O     | 38:N:18:VAL:HG22  | 2.16                     | 0.44              |
| 43:S:33:VAL:HG11 | 52:3:1272:G:H4'   | 2.00                     | 0.44              |
| 45:U:20:VAL:HG23 | 45:U:35:ARG:CA    | 2.47                     | 0.44              |
| 46:V:49:ASN:CG   | 46:V:50:ASN:N     | 2.75                     | 0.44              |
| 52:3:1256:A:O2'  | 52:3:1257:A:H5''  | 2.17                     | 0.44              |
| 53:1:2070:A:H2'  | 53:1:2071:A:O4'   | 2.17                     | 0.44              |
| 53:1:2220:U:H2'  | 53:1:2221:G:C8    | 2.51                     | 0.44              |
| 53:1:2756:U:H4'  | 53:1:2757:A:OP1   | 2.17                     | 0.44              |
| 55:5:11:A:H2'    | 55:5:12:G:C8      | 2.53                     | 0.44              |
| 5:f:44:HIS:CG    | 5:f:45:ALA:H      | 2.34                     | 0.44              |
| 8:i:21:PRO:CB    | 8:i:22:PRO:HD3    | 2.48                     | 0.44              |
| 18:s:41:LYS:HD2  | 53:1:2009:A:H5''  | 1.99                     | 0.44              |
| 18:s:42:LYS:O    | 18:s:45:VAL:HG12  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 19:t:28:ASN:HD21 | 19:t:91:GLN:HB2   | 1.81                     | 0.44              |
| 35:K:49:TYR:CE1  | 47:W:65:SER:HA    | 2.53                     | 0.44              |
| 36:L:142:ARG:NE  | 55:6:41:C:H4'     | 2.33                     | 0.44              |
| 42:R:70:ARG:O    | 42:R:74:MET:HG2   | 2.18                     | 0.44              |
| 52:3:418:C:H2'   | 52:3:419:C:C6     | 2.53                     | 0.44              |
| 53:1:171:U:H2'   | 53:1:172:A:H8     | 1.81                     | 0.44              |
| 53:1:176:A:O2'   | 53:1:177:G:H5'    | 2.17                     | 0.44              |
| 53:1:940:G:H2'   | 53:1:941:A:H5''   | 1.99                     | 0.44              |
| 53:1:2432:A:H1'  | 55:6:75:C:C5'     | 2.46                     | 0.44              |
| 53:1:2472:G:H2'  | 53:1:2475:C:H42   | 1.83                     | 0.44              |
| 54:2:29:A:H2'    | 54:2:30:C:O4'     | 2.17                     | 0.44              |
| 2:c:3:GLY:HA3    | 2:c:203:VAL:O     | 2.17                     | 0.44              |
| 4:e:35:LEU:HB2   | 4:e:88:VAL:CG2    | 2.47                     | 0.44              |
| 4:e:66:ILE:HD12  | 4:e:66:ILE:N      | 2.32                     | 0.44              |
| 4:e:140:ILE:HG22 | 4:e:142:TYR:H     | 1.83                     | 0.44              |
| 7:h:56:ARG:HE    | 7:h:83:ALA:HB2    | 1.83                     | 0.44              |
| 16:q:5:ARG:NH1   | 53:1:585:G:N7     | 2.66                     | 0.44              |
| 18:s:55:ILE:HG23 | 18:s:66:ILE:HD12  | 2.00                     | 0.44              |
| 21:v:44:HIS:NE2  | 21:v:48:MET:SD    | 2.91                     | 0.44              |
| 33:I:124:VAL:HA  | 33:I:142:VAL:HA   | 2.00                     | 0.44              |
| 35:K:29:ILE:HD11 | 35:K:66:ALA:CB    | 2.48                     | 0.44              |
| 36:L:68:VAL:HG11 | 36:L:103:ILE:HD11 | 1.98                     | 0.44              |
| 44:T:73:ASP:OD2  | 44:T:75:ALA:HB3   | 2.18                     | 0.44              |
| 51:a:60:ARG:HG3  | 51:a:164:ARG:HD3  | 1.99                     | 0.44              |
| 52:3:1023:U:H2'  | 52:3:1024:G:C8    | 2.53                     | 0.44              |
| 52:3:1333:A:H2'  | 52:3:1334:G:O4'   | 2.17                     | 0.44              |
| 53:1:213:A:H2'   | 53:1:214:G:C8     | 2.53                     | 0.44              |
| 53:1:371:A:H61   | 53:1:401:A:H3'    | 1.81                     | 0.44              |
| 53:1:2236:U:H2'  | 53:1:2237:G:O4'   | 2.18                     | 0.44              |
| 53:1:2266:A:H4'  | 53:1:2267:A:N3    | 2.32                     | 0.44              |
| 53:1:2329:U:H2'  | 53:1:2330:G:C8    | 2.52                     | 0.44              |
| 1:b:154:ALA:HB2  | 1:b:161:VAL:HG13  | 2.00                     | 0.44              |
| 6:g:114:GLU:HA   | 6:g:133:GLN:HG2   | 2.00                     | 0.44              |
| 7:h:53:ARG:HG3   | 7:h:55:VAL:HG22   | 2.00                     | 0.44              |
| 21:v:73:LYS:HG2  | 21:v:94:ALA:HB3   | 1.99                     | 0.44              |
| 24:y:42:LEU:HD23 | 24:y:45:GLN:HE21  | 1.82                     | 0.44              |
| 40:P:21:HIS:NE2  | 40:P:84:MET:SD    | 2.91                     | 0.44              |
| 44:T:3:SER:O     | 44:T:7:THR:HG23   | 2.18                     | 0.44              |
| 50:Z:25:ALA:HA   | 50:Z:28:LEU:HB2   | 1.99                     | 0.44              |
| 52:3:1001:C:H2'  | 52:3:1002:G:H8    | 1.83                     | 0.44              |
| 53:1:367:G:H2'   | 53:1:368:A:O4'    | 2.18                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:523:C:H2'   | 53:1:524:G:C8     | 2.53                     | 0.44              |
| 53:1:876:C:H2'   | 53:1:877:A:O4'    | 2.18                     | 0.44              |
| 57:7:57:G:H2'    | 57:7:58:A:H5'     | 2.00                     | 0.44              |
| 3:d:48:THR:HG23  | 3:d:50:ALA:H      | 1.82                     | 0.44              |
| 4:e:110:ILE:HB   | 4:e:113:PHE:HB2   | 1.99                     | 0.44              |
| 8:i:133:ARG:HH21 | 53:1:1078:U:H5'   | 1.82                     | 0.44              |
| 12:m:4:PRO:HG2   | 12:m:70:ASP:HA    | 2.00                     | 0.44              |
| 25:z:51:SER:HA   | 25:z:54:VAL:HG12  | 1.99                     | 0.44              |
| 29:E:17:GLY:HA3  | 53:1:651:G:H4'    | 2.00                     | 0.44              |
| 30:F:17:VAL:HG13 | 30:F:19:ARG:HG3   | 2.00                     | 0.44              |
| 36:L:62:GLU:HA   | 36:L:65:LEU:HD12  | 1.99                     | 0.44              |
| 46:V:10:ARG:HD3  | 46:V:25:GLU:OE2   | 2.18                     | 0.44              |
| 52:3:285:C:H2'   | 52:3:286:C:C6     | 2.53                     | 0.44              |
| 52:3:1015:G:H2'  | 52:3:1016:A:O4'   | 2.17                     | 0.44              |
| 52:3:1379:G:O2'  | 52:3:1380:U:H5'   | 2.17                     | 0.44              |
| 53:1:821:A:C5'   | 53:1:822:G:H5''   | 2.42                     | 0.44              |
| 53:1:995:C:H5'   | 53:1:995:C:C6     | 2.49                     | 0.44              |
| 53:1:1035:U:H2'  | 53:1:1036:G:H8    | 1.83                     | 0.44              |
| 53:1:1354:A:H2'  | 53:1:1355:G:O4'   | 2.17                     | 0.44              |
| 53:1:2515:C:H2'  | 53:1:2516:A:H8    | 1.83                     | 0.44              |
| 1:b:251:THR:OG1  | 1:b:252:LYS:N     | 2.51                     | 0.44              |
| 26:B:10:SER:OG   | 53:1:17:G:H5'     | 2.18                     | 0.44              |
| 35:K:69:GLU:HG2  | 35:K:70:VAL:N     | 2.33                     | 0.44              |
| 38:N:18:VAL:HG12 | 38:N:64:ILE:HG23  | 2.00                     | 0.44              |
| 44:T:28:VAL:HG11 | 44:T:80:LEU:HD21  | 2.00                     | 0.44              |
| 49:Y:58:ASP:OD1  | 52:3:194:C:H1'    | 2.18                     | 0.44              |
| 52:3:195:A:H2'   | 52:3:196:A:C8     | 2.53                     | 0.44              |
| 52:3:672:U:H2'   | 52:3:673:A:C8     | 2.53                     | 0.44              |
| 52:3:890:G:O2'   | 52:3:891:U:H5     | 2.00                     | 0.44              |
| 53:1:1827:U:C2'  | 53:1:1828:G:H5'   | 2.48                     | 0.44              |
| 53:1:2478:A:H2'  | 53:1:2479:U:O4'   | 2.18                     | 0.44              |
| 3:d:63:LYS:HD3   | 53:1:2443:C:OP1   | 2.18                     | 0.43              |
| 31:G:153:MET:HE1 | 31:G:155:GLY:O    | 2.18                     | 0.43              |
| 31:G:156:LEU:O   | 31:G:156:LEU:HD12 | 2.18                     | 0.43              |
| 36:L:21:LEU:HD23 | 36:L:21:LEU:H     | 1.83                     | 0.43              |
| 38:N:49:GLN:N    | 38:N:50:PRO:HD2   | 2.33                     | 0.43              |
| 44:T:84:LEU:HG   | 44:T:86:LEU:HD13  | 1.99                     | 0.43              |
| 46:V:64:ARG:HD2  | 52:3:264:C:H4'    | 1.99                     | 0.43              |
| 47:W:59:LYS:HA   | 47:W:62:ARG:HB2   | 2.00                     | 0.43              |
| 52:3:162:A:H2'   | 52:3:163:C:O4'    | 2.18                     | 0.43              |
| 53:1:225:C:H2'   | 53:1:226:A:O4'    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:664:G:H4'   | 53:1:941:A:OP1    | 2.18                     | 0.43              |
| 53:1:2328:A:H2'  | 53:1:2329:U:C6    | 2.52                     | 0.43              |
| 53:1:2359:C:H2'  | 53:1:2360:G:C8    | 2.53                     | 0.43              |
| 53:1:2359:C:H2'  | 53:1:2360:G:H8    | 1.83                     | 0.43              |
| 12:m:45:GLN:NE2  | 53:1:2485:G:H5''  | 2.33                     | 0.43              |
| 18:s:11:ARG:HD3  | 18:s:11:ARG:N     | 2.33                     | 0.43              |
| 31:G:22:TRP:HE1  | 52:3:830:G:H5'    | 1.82                     | 0.43              |
| 32:H:78:LYS:C    | 32:H:79:LYS:HG3   | 2.43                     | 0.43              |
| 35:K:91:ARG:HD3  | 52:3:738:C:OP2    | 2.18                     | 0.43              |
| 36:L:15:PRO:HB2  | 38:N:44:ARG:HH12  | 1.83                     | 0.43              |
| 39:O:41:PRO:HG3  | 52:3:1150:A:C2    | 2.52                     | 0.43              |
| 40:P:80:ASN:HB3  | 40:P:105:ARG:HB3  | 1.99                     | 0.43              |
| 48:X:14:LEU:HD23 | 48:X:37:SER:OG    | 2.17                     | 0.43              |
| 50:Z:36:PHE:O    | 50:Z:37:TYR:HB2   | 2.17                     | 0.43              |
| 53:1:577:G:OP1   | 53:1:2502:G:H2'   | 2.18                     | 0.43              |
| 53:1:644:A:H61   | 53:1:2349:G:N2    | 2.15                     | 0.43              |
| 53:1:968:C:H2'   | 53:1:969:G:C8     | 2.52                     | 0.43              |
| 53:1:1709:U:H2'  | 53:1:1710:G:C8    | 2.54                     | 0.43              |
| 53:1:2019:A:H2   | 53:1:2035:G:H22   | 1.66                     | 0.43              |
| 53:1:2494:G:H2'  | 53:1:2495:G:C8    | 2.53                     | 0.43              |
| 4:e:7:TYR:HB2    | 4:e:172:PHE:HZ    | 1.83                     | 0.43              |
| 4:e:111:ARG:HH11 | 42:R:6:ILE:HG23   | 1.83                     | 0.43              |
| 17:r:52:PRO:O    | 17:r:53:PHE:CB    | 2.65                     | 0.43              |
| 23:x:63:ILE:HD12 | 23:x:63:ILE:N     | 2.30                     | 0.43              |
| 32:H:173:PRO:O   | 32:H:181:ILE:HD11 | 2.18                     | 0.43              |
| 33:I:186:GLU:HB2 | 33:I:189:ASP:OD1  | 2.18                     | 0.43              |
| 33:I:187:ARG:NH2 | 33:I:194:ILE:O    | 2.51                     | 0.43              |
| 38:N:41:GLU:O    | 38:N:44:ARG:NE    | 2.52                     | 0.43              |
| 45:U:33:ILE:HD12 | 45:U:33:ILE:N     | 2.33                     | 0.43              |
| 47:W:11:ARG:H    | 47:W:11:ARG:HD3   | 1.83                     | 0.43              |
| 49:Y:34:VAL:O    | 49:Y:38:ILE:HG13  | 2.18                     | 0.43              |
| 52:3:335:C:H2'   | 52:3:336:A:C8     | 2.54                     | 0.43              |
| 53:1:1636:U:H2'  | 53:1:1637:A:C8    | 2.53                     | 0.43              |
| 53:1:1827:U:H2'  | 53:1:1828:G:O4'   | 2.18                     | 0.43              |
| 53:1:2710:C:H2'  | 53:1:2711:A:H8    | 1.83                     | 0.43              |
| 3:d:1:MET:HG3    | 3:d:16:GLU:HA     | 2.00                     | 0.43              |
| 12:m:73:ILE:HD12 | 12:m:73:ILE:HA    | 1.92                     | 0.43              |
| 20:u:73:ASN:ND2  | 20:u:75:ALA:HB3   | 2.34                     | 0.43              |
| 22:w:38:GLY:HA2  | 53:1:2330:G:H21   | 1.84                     | 0.43              |
| 28:D:45:SER:OG   | 28:D:46:LYS:N     | 2.49                     | 0.43              |
| 30:F:22:VAL:HG13 | 30:F:37:GLN:OE1   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 38:N:4:GLN:HE22  | 52:3:1131:G:H5'   | 1.83                     | 0.43              |
| 41:Q:2:THR:CG2   | 41:Q:5:GLN:HG3    | 2.48                     | 0.43              |
| 41:Q:23:LEU:HD12 | 41:Q:23:LEU:HA    | 1.79                     | 0.43              |
| 41:Q:81:ILE:HD11 | 41:Q:94:TYR:CB    | 2.48                     | 0.43              |
| 53:1:249:C:H2'   | 53:1:2394:C:O2'   | 2.18                     | 0.43              |
| 53:1:780:G:H2'   | 53:1:782:A:N7     | 2.33                     | 0.43              |
| 53:1:2489:U:H2'  | 53:1:2490:G:O4'   | 2.18                     | 0.43              |
| 55:6:36:U:H2'    | 55:6:37:A:H5'     | 2.00                     | 0.43              |
| 1:b:77:VAL:HA    | 1:b:93:VAL:HA     | 2.01                     | 0.43              |
| 2:c:56:LYS:NZ    | 53:1:2830:C:H5''  | 2.34                     | 0.43              |
| 3:d:157:LEU:HG   | 3:d:169:VAL:HG11  | 2.00                     | 0.43              |
| 4:e:39:VAL:HG13  | 4:e:40:GLY:H      | 1.82                     | 0.43              |
| 4:e:174:PHE:HA   | 4:e:175:PRO:HD3   | 1.84                     | 0.43              |
| 6:g:51:ARG:HA    | 6:g:55:GLU:HB2    | 2.00                     | 0.43              |
| 8:i:99:LYS:C     | 8:i:99:LYS:HD3    | 2.44                     | 0.43              |
| 12:m:74:THR:OG1  | 12:m:75:GLU:N     | 2.51                     | 0.43              |
| 13:n:55:ALA:HA   | 13:n:80:PHE:CE1   | 2.53                     | 0.43              |
| 20:u:81:ARG:O    | 20:u:96:LYS:HG2   | 2.18                     | 0.43              |
| 32:H:115:VAL:O   | 32:H:119:ILE:HG12 | 2.18                     | 0.43              |
| 34:J:121:ASN:HB2 | 34:J:122:VAL:H    | 1.52                     | 0.43              |
| 36:L:78:ARG:HB3  | 36:L:83:THR:HB    | 2.00                     | 0.43              |
| 36:L:78:ARG:NH1  | 52:3:1382:C:H4'   | 2.33                     | 0.43              |
| 37:M:3:GLN:O     | 52:3:587:G:H4'    | 2.19                     | 0.43              |
| 43:S:20:PHE:C    | 43:S:22:LYS:H     | 2.25                     | 0.43              |
| 52:3:868:C:H2'   | 52:3:869:G:O4'    | 2.18                     | 0.43              |
| 52:3:1016:A:H4'  | 52:3:1218:C:H4'   | 1.99                     | 0.43              |
| 52:3:1391:U:H2'  | 52:3:1392:G:C8    | 2.54                     | 0.43              |
| 53:1:84:A:H4'    | 53:1:85:G:O5'     | 2.18                     | 0.43              |
| 53:1:118:A:OP2   | 53:1:119:A:H5''   | 2.18                     | 0.43              |
| 53:1:523:C:H2'   | 53:1:524:G:H8     | 1.83                     | 0.43              |
| 53:1:1204:A:H4'  | 53:1:1205:A:H5''  | 2.00                     | 0.43              |
| 53:1:1736:U:H2'  | 53:1:1737:G:O4'   | 2.19                     | 0.43              |
| 53:1:1991:U:H2'  | 53:1:1992:G:H5''  | 1.99                     | 0.43              |
| 3:d:47:LYS:HE2   | 3:d:51:GLU:HG2    | 2.00                     | 0.43              |
| 5:f:2:ARG:HD3    | 53:1:2751:G:C4    | 2.53                     | 0.43              |
| 9:j:49:ASP:HB2   | 9:j:114:LEU:HD11  | 2.01                     | 0.43              |
| 12:m:29:GLY:HA2  | 12:m:106:ASP:HB2  | 2.01                     | 0.43              |
| 14:o:101:GLY:HA3 | 54:2:49:C:OP1     | 2.19                     | 0.43              |
| 42:R:97:ARG:HB2  | 42:R:99:GLN:OE1   | 2.18                     | 0.43              |
| 43:S:8:ARG:HG2   | 43:S:12:ARG:NH1   | 2.34                     | 0.43              |
| 49:Y:43:LYS:HB3  | 49:Y:85:LEU:HG    | 1.99                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 52:3:439:U:H2'    | 52:3:440:C:O4'   | 2.19                     | 0.43              |
| 52:3:1271:A:H5'   | 52:3:1314:C:H5'' | 1.99                     | 0.43              |
| 53:1:176:A:H3'    | 53:1:177:G:H21   | 1.83                     | 0.43              |
| 53:1:562:U:O4'    | 53:1:2036:C:H5'  | 2.18                     | 0.43              |
| 53:1:1148:U:H2'   | 53:1:1149:G:C8   | 2.53                     | 0.43              |
| 53:1:1779:U:H5    | 53:1:1784:A:N7   | 2.17                     | 0.43              |
| 53:1:2861:U:H2'   | 53:1:2862:G:H8   | 1.82                     | 0.43              |
| 1:b:48:ILE:HD11   | 1:b:51:ARG:HA    | 2.01                     | 0.43              |
| 36:L:3:ARG:HG2    | 36:L:4:ARG:HH21  | 1.83                     | 0.43              |
| 36:L:68:VAL:HA    | 36:L:137:ARG:HD3 | 2.00                     | 0.43              |
| 36:L:87:PRO:HG3   | 36:L:148:LYS:HA  | 2.01                     | 0.43              |
| 38:N:49:GLN:O     | 38:N:52:GLU:HG2  | 2.19                     | 0.43              |
| 38:N:112:ARG:HH12 | 52:3:1187:G:H4'  | 1.83                     | 0.43              |
| 43:S:29:ILE:HD12  | 43:S:29:ILE:H    | 1.83                     | 0.43              |
| 53:1:1070:A:H2'   | 53:1:1097:U:OP1  | 2.18                     | 0.43              |
| 53:1:2475:C:H2'   | 53:1:2476:A:H5'  | 2.00                     | 0.43              |
| 2:c:70:LYS:HD2    | 2:c:70:LYS:HA    | 1.90                     | 0.43              |
| 6:g:116:ARG:O     | 6:g:118:PRO:HD3  | 2.17                     | 0.43              |
| 9:j:32:LEU:HD21   | 9:j:56:VAL:HG21  | 1.99                     | 0.43              |
| 17:r:40:MET:SD    | 17:r:41:ILE:N    | 2.91                     | 0.43              |
| 33:I:111:ALA:HB1  | 52:3:407:U:H5''  | 2.01                     | 0.43              |
| 36:L:33:GLY:HA3   | 52:3:1350:A:H2   | 1.84                     | 0.43              |
| 44:T:31:LEU:HD22  | 44:T:58:MET:HB2  | 2.00                     | 0.43              |
| 47:W:36:GLY:HA3   | 47:W:70:THR:HA   | 2.01                     | 0.43              |
| 52:3:24:U:H2'     | 52:3:25:C:C6     | 2.54                     | 0.43              |
| 53:1:253:C:H2'    | 53:1:254:G:O4'   | 2.19                     | 0.43              |
| 53:1:370:G:H2'    | 53:1:423:A:N7    | 2.33                     | 0.43              |
| 53:1:755:U:H2'    | 53:1:756:A:C8    | 2.53                     | 0.43              |
| 53:1:1772:A:H2'   | 53:1:1773:A:H4'  | 2.00                     | 0.43              |
| 53:1:2326:C:O2'   | 53:1:2327:A:OP1  | 2.35                     | 0.43              |
| 53:1:2552:U:C6    | 53:1:2554:U:H5'  | 2.54                     | 0.43              |
| 53:1:2691:C:H2'   | 53:1:2692:G:C8   | 2.54                     | 0.43              |
| 53:1:2699:C:H2'   | 53:1:2700:A:H8   | 1.84                     | 0.43              |
| 4:e:118:ALA:C     | 4:e:119:LYS:HD3  | 2.44                     | 0.43              |
| 6:g:97:ARG:HG2    | 6:g:112:LYS:CD   | 2.49                     | 0.43              |
| 7:h:118:ILE:HB    | 7:h:119:PRO:HD3  | 2.01                     | 0.43              |
| 11:l:118:THR:HA   | 11:l:119:PRO:HD3 | 1.89                     | 0.43              |
| 16:q:80:ASN:CG    | 53:1:1151:A:H4'  | 2.44                     | 0.43              |
| 32:H:30:ASP:HA    | 43:S:64:ARG:HH12 | 1.84                     | 0.43              |
| 32:H:112:ALA:HB2  | 32:H:182:ASP:HB3 | 1.99                     | 0.43              |
| 39:O:53:ILE:HG23  | 52:3:1060:U:H4'  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 40:P:87:GLY:H    | 40:P:113:THR:HG22 | 1.83                     | 0.43              |
| 45:U:79:ASN:O    | 45:U:80:LYS:HE2   | 2.19                     | 0.43              |
| 47:W:70:THR:HG22 | 47:W:73:HIS:CE1   | 2.53                     | 0.43              |
| 52:3:434:U:H2'   | 52:3:435:A:C8     | 2.54                     | 0.43              |
| 52:3:1199:U:H2'  | 52:3:1200:C:H5'   | 2.01                     | 0.43              |
| 53:1:940:G:C3'   | 53:1:941:A:H5''   | 2.49                     | 0.43              |
| 53:1:1279:G:H2'  | 53:1:1280:G:H8    | 1.83                     | 0.43              |
| 53:1:2128:G:H1'  | 53:1:2173:A:N3    | 2.33                     | 0.43              |
| 53:1:2360:G:C2'  | 53:1:2361:G:H5'   | 2.48                     | 0.43              |
| 6:g:25:TYR:O     | 6:g:30:LEU:HD13   | 2.18                     | 0.43              |
| 9:j:32:LEU:O     | 9:j:36:LEU:HD13   | 2.19                     | 0.43              |
| 12:m:78:LEU:HD11 | 53:1:2459:A:C2    | 2.54                     | 0.43              |
| 14:o:87:ILE:HG22 | 14:o:90:VAL:HG22  | 2.01                     | 0.43              |
| 19:t:8:LEU:HD21  | 19:t:50:LEU:HD21  | 2.01                     | 0.43              |
| 21:v:26:PHE:HE2  | 21:v:89:ILE:HG12  | 1.83                     | 0.43              |
| 33:I:23:GLY:HA3  | 52:3:409:U:OP1    | 2.19                     | 0.43              |
| 36:L:16:LYS:HD2  | 36:L:17:PHE:HD1   | 1.84                     | 0.43              |
| 52:3:32:A:H2'    | 52:3:33:A:C8      | 2.54                     | 0.43              |
| 52:3:86:G:H4'    | 52:3:87:C:C5      | 2.54                     | 0.43              |
| 52:3:366:A:H2    | 52:3:394:G:H1     | 1.65                     | 0.43              |
| 52:3:824:G:H2'   | 52:3:825:A:H8     | 1.83                     | 0.43              |
| 52:3:1429:A:O2'  | 52:3:1430:A:H5'   | 2.19                     | 0.43              |
| 53:1:112:U:C2'   | 53:1:113:U:H5'    | 2.48                     | 0.43              |
| 53:1:341:C:H2'   | 53:1:342:A:C8     | 2.53                     | 0.43              |
| 53:1:1806:C:H2'  | 53:1:1807:G:O4'   | 2.19                     | 0.43              |
| 53:1:2457:U:O2'  | 53:1:2458:G:H5'   | 2.19                     | 0.43              |
| 57:7:47:U:H3'    | 57:7:48:C:C5'     | 2.49                     | 0.43              |
| 7:h:93:ALA:HB3   | 7:h:95:LEU:HD12   | 2.01                     | 0.42              |
| 10:k:93:GLN:HA   | 10:k:94:PRO:HD2   | 1.85                     | 0.42              |
| 39:O:63:ASP:OD2  | 39:O:63:ASP:N     | 2.50                     | 0.42              |
| 42:R:96:VAL:HG12 | 52:3:1308:U:OP1   | 2.19                     | 0.42              |
| 45:U:69:ASP:OD2  | 45:U:70:ARG:N     | 2.52                     | 0.42              |
| 52:3:1032:G:H3'  | 52:3:1032:G:N3    | 2.34                     | 0.42              |
| 53:1:12:U:O2'    | 53:1:13:A:H5'     | 2.19                     | 0.42              |
| 53:1:123:G:H2'   | 53:1:124:G:O4'    | 2.17                     | 0.42              |
| 53:1:306:U:H2'   | 53:1:307:G:O4'    | 2.19                     | 0.42              |
| 53:1:441:U:H2'   | 53:1:442:G:C8     | 2.54                     | 0.42              |
| 53:1:598:U:H2'   | 53:1:599:A:C8     | 2.54                     | 0.42              |
| 5:f:44:HIS:O     | 5:f:45:ALA:HB3    | 2.19                     | 0.42              |
| 9:j:7:LYS:HA     | 9:j:8:PRO:HD3     | 1.84                     | 0.42              |
| 9:j:113:PRO:HD2  | 53:1:558:U:OP1    | 2.18                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 12:m:42:THR:OG1   | 12:m:45:GLN:HG3  | 2.19                     | 0.42              |
| 35:K:47:LEU:HD13  | 35:K:51:ILE:HG22 | 2.00                     | 0.42              |
| 36:L:29:LEU:HD23  | 36:L:29:LEU:O    | 2.19                     | 0.42              |
| 37:M:103:VAL:HA   | 37:M:124:ILE:HA  | 2.01                     | 0.42              |
| 40:P:116:PRO:HB3  | 52:3:676:A:H1'   | 2.01                     | 0.42              |
| 50:Z:57:LYS:HA    | 50:Z:60:ALA:HB3  | 2.01                     | 0.42              |
| 52:3:10:A:H2'     | 52:3:11:G:C8     | 2.55                     | 0.42              |
| 52:3:361:G:H2'    | 52:3:362:G:O4'   | 2.20                     | 0.42              |
| 52:3:604:G:H2'    | 52:3:605:U:O4'   | 2.20                     | 0.42              |
| 52:3:1118:U:H2'   | 52:3:1119:C:C6   | 2.53                     | 0.42              |
| 53:1:214:G:H2'    | 53:1:215:G:C8    | 2.54                     | 0.42              |
| 53:1:668:A:H2'    | 53:1:670:A:H62   | 1.84                     | 0.42              |
| 53:1:1153:C:H2'   | 53:1:1154:G:O4'  | 2.19                     | 0.42              |
| 53:1:2512:C:H2'   | 53:1:2513:A:O4'  | 2.18                     | 0.42              |
| 53:1:2670:A:H2'   | 53:1:2671:G:C8   | 2.53                     | 0.42              |
| 53:1:2743:U:H2'   | 53:1:2744:G:C4'  | 2.49                     | 0.42              |
| 4:e:68:LYS:HB3    | 4:e:81:GLY:HA2   | 2.00                     | 0.42              |
| 9:j:36:LEU:HD21   | 9:j:122:LEU:HB2  | 2.02                     | 0.42              |
| 11:l:119:PRO:HG3  | 11:l:138:ALA:O   | 2.20                     | 0.42              |
| 19:t:69:ARG:NH2   | 53:1:1334:G:H5'' | 2.33                     | 0.42              |
| 35:K:36:ILE:N     | 35:K:36:ILE:HD12 | 2.34                     | 0.42              |
| 42:R:103:THR:HG22 | 52:3:1229:A:H61  | 1.84                     | 0.42              |
| 44:T:7:THR:HG21   | 52:3:659:U:OP1   | 2.18                     | 0.42              |
| 48:X:9:PHE:CD2    | 52:3:1318:A:H4'  | 2.54                     | 0.42              |
| 52:3:150:U:H3     | 52:3:171:A:H62   | 1.67                     | 0.42              |
| 52:3:390:U:H2'    | 52:3:391:G:C8    | 2.54                     | 0.42              |
| 52:3:858:G:O6     | 52:3:869:G:H3'   | 2.19                     | 0.42              |
| 52:3:1280:A:O2'   | 52:3:1281:C:H5'  | 2.18                     | 0.42              |
| 53:1:2163:A:H2'   | 53:1:2164:C:H5'  | 2.00                     | 0.42              |
| 53:1:2196:C:O2'   | 53:1:2197:U:H5'  | 2.19                     | 0.42              |
| 53:1:2358:A:H2'   | 53:1:2359:C:O4'  | 2.19                     | 0.42              |
| 53:1:2370:G:H2'   | 53:1:2371:G:O4'  | 2.19                     | 0.42              |
| 53:1:2446:G:H2'   | 53:1:2447:G:H5'' | 2.00                     | 0.42              |
| 53:1:2665:A:O2'   | 53:1:2666:C:H5'  | 2.19                     | 0.42              |
| 53:1:2788:C:H2'   | 53:1:2789:C:C6   | 2.54                     | 0.42              |
| 4:e:107:VAL:O     | 4:e:110:ILE:HD12 | 2.20                     | 0.42              |
| 7:h:29:ASP:O      | 7:h:56:ARG:NH1   | 2.52                     | 0.42              |
| 7:h:112:ALA:O     | 7:h:113:PHE:C    | 2.62                     | 0.42              |
| 11:l:93:ASN:C     | 11:l:95:LEU:H    | 2.28                     | 0.42              |
| 12:m:3:GLN:HA     | 12:m:4:PRO:HD3   | 1.89                     | 0.42              |
| 12:m:50:ARG:HA    | 12:m:53:MET:HE2  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 32:H:170:GLY:O   | 52:3:1106:G:H4'  | 2.19                     | 0.42              |
| 33:I:123:MET:HB3 | 33:I:128:VAL:HA  | 2.00                     | 0.42              |
| 34:J:83:PRO:HB3  | 34:J:96:GLN:HG3  | 2.00                     | 0.42              |
| 34:J:108:GLY:O   | 34:J:109:ALA:HB3 | 2.19                     | 0.42              |
| 38:N:30:ASN:C    | 38:N:32:ARG:H    | 2.27                     | 0.42              |
| 41:Q:15:VAL:HG13 | 41:Q:15:VAL:O    | 2.19                     | 0.42              |
| 41:Q:113:ARG:HD2 | 41:Q:118:VAL:O   | 2.19                     | 0.42              |
| 46:V:42:LYS:HD2  | 52:3:278:G:OP2   | 2.19                     | 0.42              |
| 51:a:33:LEU:HD13 | 51:a:220:ALA:H   | 1.85                     | 0.42              |
| 52:3:79:G:H2'    | 52:3:80:A:O4'    | 2.19                     | 0.42              |
| 52:3:225:C:H2'   | 52:3:226:G:O4'   | 2.20                     | 0.42              |
| 52:3:304:U:O2'   | 52:3:305:G:H5'   | 2.20                     | 0.42              |
| 53:1:560:C:H2'   | 53:1:561:G:O4'   | 2.18                     | 0.42              |
| 53:1:859:G:C2'   | 53:1:860:U:OP2   | 2.66                     | 0.42              |
| 53:1:1432:G:H2'  | 53:1:1433:A:C8   | 2.55                     | 0.42              |
| 53:1:1525:A:H2'  | 53:1:1526:C:O4'  | 2.19                     | 0.42              |
| 53:1:1837:C:H2'  | 53:1:1899:A:N6   | 2.34                     | 0.42              |
| 53:1:2112:G:H2'  | 53:1:2113:U:H5'  | 2.00                     | 0.42              |
| 54:2:117:G:H2'   | 54:2:118:C:O4'   | 2.19                     | 0.42              |
| 1:b:237:ARG:HD2  | 53:1:2591:C:OP1  | 2.20                     | 0.42              |
| 1:b:261:ARG:NH2  | 53:1:1801:A:C4   | 2.87                     | 0.42              |
| 3:d:68:ALA:HA    | 53:1:1255:U:C5   | 2.54                     | 0.42              |
| 3:d:105:LEU:HA   | 3:d:108:ILE:HG22 | 2.02                     | 0.42              |
| 4:e:37:MET:HB2   | 4:e:86:CYS:SG    | 2.60                     | 0.42              |
| 25:z:35:VAL:HG22 | 25:z:36:GLU:H    | 1.85                     | 0.42              |
| 32:H:175:HIS:ND1 | 52:3:1108:G:H5'  | 2.34                     | 0.42              |
| 36:L:74:VAL:HG21 | 36:L:85:GLN:HB3  | 2.01                     | 0.42              |
| 52:3:243:A:H4'   | 52:3:244:U:H3'   | 2.02                     | 0.42              |
| 52:3:701:U:C4'   | 52:3:703:G:H1'   | 2.47                     | 0.42              |
| 53:1:28:A:O2'    | 53:1:583:G:H5'   | 2.19                     | 0.42              |
| 53:1:341:C:H2'   | 53:1:342:A:H8    | 1.84                     | 0.42              |
| 53:1:854:C:H2'   | 53:1:855:G:C8    | 2.53                     | 0.42              |
| 53:1:1319:C:O2'  | 53:1:1320:C:H5'  | 2.19                     | 0.42              |
| 53:1:1366:A:H2'  | 53:1:1367:A:O4'  | 2.19                     | 0.42              |
| 53:1:1370:C:H2'  | 53:1:1371:G:O4'  | 2.19                     | 0.42              |
| 13:n:79:LEU:C    | 13:n:81:ASN:H    | 2.28                     | 0.42              |
| 14:o:53:THR:HB   | 14:o:65:THR:HB   | 2.02                     | 0.42              |
| 19:t:21:SER:O    | 19:t:24:MET:HB3  | 2.19                     | 0.42              |
| 23:x:63:ILE:O    | 23:x:67:LEU:HD23 | 2.19                     | 0.42              |
| 33:I:77:GLU:O    | 33:I:81:LEU:HD23 | 2.19                     | 0.42              |
| 36:L:2:ARG:HB3   | 52:3:933:G:OP2   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 36:L:14:ASP:OD1  | 36:L:15:PRO:HD2  | 2.19                     | 0.42              |
| 41:Q:40:THR:HA   | 41:Q:41:PRO:HD3  | 1.78                     | 0.42              |
| 52:3:312:C:H2'   | 52:3:313:A:C8    | 2.54                     | 0.42              |
| 53:1:275:C:H3'   | 53:1:276:U:H5''  | 2.02                     | 0.42              |
| 53:1:391:A:H2'   | 53:1:391:A:N3    | 2.34                     | 0.42              |
| 53:1:438:G:H2'   | 53:1:439:A:C8    | 2.55                     | 0.42              |
| 53:1:742:A:H2'   | 53:1:743:A:H8    | 1.84                     | 0.42              |
| 53:1:873:C:H2'   | 53:1:874:G:H8    | 1.83                     | 0.42              |
| 53:1:1474:U:H2'  | 53:1:1475:G:H5'  | 2.00                     | 0.42              |
| 53:1:2329:U:H2'  | 53:1:2330:G:H8   | 1.83                     | 0.42              |
| 57:7:47:U:H3'    | 57:7:48:C:H5''   | 2.01                     | 0.42              |
| 6:g:49:ALA:O     | 6:g:53:GLU:HB2   | 2.20                     | 0.42              |
| 7:h:129:LEU:HA   | 7:h:130:PRO:HD3  | 1.89                     | 0.42              |
| 11:l:17:LYS:HE3  | 11:l:27:LEU:HD11 | 2.02                     | 0.42              |
| 13:n:6:SER:H     | 53:1:2873:A:H2   | 1.68                     | 0.42              |
| 19:t:76:ARG:HH22 | 53:1:57:C:H3'    | 1.85                     | 0.42              |
| 22:w:47:VAL:HG21 | 22:w:76:ILE:O    | 2.19                     | 0.42              |
| 26:B:24:VAL:HG23 | 26:B:25:THR:N    | 2.34                     | 0.42              |
| 33:I:82:LYS:HG2  | 33:I:83:GLY:H    | 1.84                     | 0.42              |
| 40:P:12:ARG:O    | 40:P:13:LYS:HG2  | 2.19                     | 0.42              |
| 40:P:62:ALA:HB1  | 40:P:95:THR:HB   | 2.01                     | 0.42              |
| 42:R:55:LEU:O    | 42:R:55:LEU:HD23 | 2.19                     | 0.42              |
| 43:S:72:PHE:C    | 43:S:73:LEU:HD12 | 2.44                     | 0.42              |
| 44:T:25:GLU:O    | 44:T:28:VAL:HG12 | 2.20                     | 0.42              |
| 51:a:54:LYS:HB2  | 51:a:57:GLN:HB2  | 2.01                     | 0.42              |
| 52:3:1319:A:H4'  | 52:3:1320:C:H5   | 1.83                     | 0.42              |
| 53:1:123:G:O2'   | 53:1:1376:C:H4'  | 2.20                     | 0.42              |
| 53:1:1179:G:N7   | 53:1:1180:U:H1'  | 2.35                     | 0.42              |
| 53:1:1955:U:C4   | 53:1:2552:U:H1'  | 2.55                     | 0.42              |
| 53:1:2139:U:H2'  | 53:1:2140:G:C8   | 2.54                     | 0.42              |
| 53:1:2286:G:H4'  | 53:1:2287:A:O5'  | 2.18                     | 0.42              |
| 53:1:2317:A:H2'  | 53:1:2318:G:O4'  | 2.19                     | 0.42              |
| 53:1:2628:C:H3'  | 53:1:2629:U:C5'  | 2.50                     | 0.42              |
| 1:b:91:ALA:HB2   | 1:b:105:ALA:HB2  | 2.02                     | 0.42              |
| 1:b:234:GLY:HA3  | 1:b:238:ASN:HD22 | 1.84                     | 0.42              |
| 6:g:8:LYS:HZ2    | 6:g:14:SER:C     | 2.28                     | 0.42              |
| 15:p:105:LYS:HD3 | 15:p:108:ARG:NH1 | 2.34                     | 0.42              |
| 24:y:2:LYS:HG3   | 24:y:3:ALA:N     | 2.34                     | 0.42              |
| 30:F:32:LYS:CE   | 53:1:2478:A:H5'  | 2.50                     | 0.42              |
| 37:M:17:GLN:HG2  | 37:M:62:LEU:HD13 | 2.01                     | 0.42              |
| 38:N:12:LYS:HD2  | 38:N:12:LYS:O    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-----------------|--------------------------|-------------------|
| 40:P:35:ASP:OD1   | 40:P:39:ASN:N   | 2.53                     | 0.42              |
| 52:3:1258:G:H2'   | 52:3:1259:C:C6  | 2.54                     | 0.42              |
| 53:1:248:G:H3'    | 53:1:249:C:C5'  | 2.49                     | 0.42              |
| 53:1:248:G:H3'    | 53:1:249:C:H5'' | 2.00                     | 0.42              |
| 53:1:406:G:H2'    | 53:1:407:G:C8   | 2.55                     | 0.42              |
| 53:1:415:A:H2'    | 53:1:416:U:C6   | 2.55                     | 0.42              |
| 53:1:488:G:H22    | 53:1:491:G:H5'' | 1.85                     | 0.42              |
| 53:1:871:U:H2'    | 53:1:872:U:C6   | 2.54                     | 0.42              |
| 53:1:1130:U:O2'   | 53:1:1131:G:OP1 | 2.33                     | 0.42              |
| 53:1:1130:U:O2'   | 53:1:1131:G:P   | 2.78                     | 0.42              |
| 53:1:1683:U:H2'   | 53:1:1684:G:H8  | 1.85                     | 0.42              |
| 53:1:2484:G:O2'   | 53:1:2485:G:H5' | 2.20                     | 0.42              |
| 55:5:21:A:H61     | 55:5:46:G:H2'   | 1.84                     | 0.42              |
| 1:b:97:ASP:HB3    | 53:1:1490:A:N7  | 2.34                     | 0.42              |
| 1:b:220:ARG:NH1   | 53:1:1827:U:OP2 | 2.52                     | 0.42              |
| 3:d:146:VAL:HG22  | 3:d:147:LEU:N   | 2.34                     | 0.42              |
| 3:d:176:ASP:HA    | 3:d:177:PRO:HD3 | 1.85                     | 0.42              |
| 4:e:7:TYR:O       | 4:e:12:VAL:HG23 | 2.20                     | 0.42              |
| 14:o:94:ARG:HD2   | 53:1:2376:A:N6  | 2.35                     | 0.42              |
| 18:s:79:GLY:N     | 18:s:101:SER:HA | 2.33                     | 0.42              |
| 18:s:83:LYS:HG2   | 18:s:95:ARG:NH1 | 2.32                     | 0.42              |
| 37:M:105:THR:OG1  | 37:M:106:SER:N  | 2.52                     | 0.42              |
| 41:Q:2:THR:HG22   | 41:Q:5:GLN:HG3  | 2.01                     | 0.42              |
| 51:a:212:VAL:HG13 | 51:a:224:VAL:HB | 2.02                     | 0.42              |
| 53:1:135:U:H2'    | 53:1:136:G:C8   | 2.54                     | 0.42              |
| 53:1:277:G:H4'    | 53:1:278:A:N7   | 2.35                     | 0.42              |
| 53:1:596:U:H2'    | 53:1:597:G:C8   | 2.54                     | 0.42              |
| 53:1:1474:U:C2'   | 53:1:1475:G:H5' | 2.50                     | 0.42              |
| 53:1:1930:G:O2'   | 53:1:1931:U:C5  | 2.71                     | 0.42              |
| 2:c:101:PHE:HE1   | 2:c:205:PRO:HD3 | 1.85                     | 0.42              |
| 7:h:81:LEU:HD21   | 53:1:1106:G:N2  | 2.33                     | 0.42              |
| 14:o:5:SER:O      | 14:o:8:ILE:HG22 | 2.20                     | 0.42              |
| 17:r:78:ARG:HB2   | 17:r:83:TYR:HD2 | 1.85                     | 0.42              |
| 20:u:44:HIS:HB2   | 53:1:482:A:H4'  | 2.01                     | 0.42              |
| 29:E:60:CYS:O     | 29:E:62:PRO:HD3 | 2.20                     | 0.42              |
| 53:1:230:G:O2'    | 53:1:231:A:H5'  | 2.20                     | 0.42              |
| 53:1:1071:G:OP1   | 53:1:1071:G:H3' | 2.20                     | 0.42              |
| 53:1:1231:U:H2'   | 53:1:1232:G:H8  | 1.85                     | 0.42              |
| 54:2:5:U:H2'      | 54:2:6:G:C8     | 2.55                     | 0.42              |
| 2:c:4:LEU:HD22    | 2:c:32:ASN:ND2  | 2.35                     | 0.41              |
| 3:d:90:GLN:HG3    | 3:d:92:HIS:CE1  | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:e:70:ARG:NH2    | 53:1:2298:A:OP1   | 2.53                     | 0.41              |
| 21:v:17:SER:O     | 21:v:20:LEU:HD23  | 2.20                     | 0.41              |
| 41:Q:42:LYS:NZ    | 52:3:912:C:H5''   | 2.35                     | 0.41              |
| 43:S:60:ARG:HA    | 43:S:60:ARG:HD2   | 1.76                     | 0.41              |
| 44:T:54:GLY:O     | 44:T:57:ARG:HB3   | 2.20                     | 0.41              |
| 45:U:67:ILE:HG22  | 45:U:71:VAL:HG13  | 2.02                     | 0.41              |
| 52:3:17:U:H2'     | 52:3:18:C:C6      | 2.55                     | 0.41              |
| 52:3:326:G:H2'    | 52:3:327:A:H5'    | 2.02                     | 0.41              |
| 52:3:335:C:H2'    | 52:3:336:A:H8     | 1.85                     | 0.41              |
| 52:3:948:C:H2'    | 52:3:949:A:H8     | 1.85                     | 0.41              |
| 53:1:687:C:H6     | 53:1:687:C:H5'    | 1.85                     | 0.41              |
| 53:1:738:G:O2'    | 53:1:739:A:H5'    | 2.20                     | 0.41              |
| 53:1:741:U:H2'    | 53:1:742:A:H8     | 1.85                     | 0.41              |
| 53:1:967:U:H2'    | 53:1:968:C:C6     | 2.55                     | 0.41              |
| 53:1:1496:A:H2'   | 53:1:1498:C:N4    | 2.35                     | 0.41              |
| 53:1:1558:C:H4'   | 53:1:1560:G:OP2   | 2.20                     | 0.41              |
| 53:1:1846:G:H2'   | 53:1:1847:A:O4'   | 2.20                     | 0.41              |
| 53:1:1965:C:H5''  | 53:1:1966:A:H2'   | 2.02                     | 0.41              |
| 54:2:28:C:H2'     | 54:2:29:A:C8      | 2.55                     | 0.41              |
| 54:2:97:C:H2'     | 54:2:98:G:H5'     | 2.02                     | 0.41              |
| 1:b:224:MET:SD    | 1:b:229:HIS:HB2   | 2.60                     | 0.41              |
| 1:b:245:THR:OG1   | 1:b:246:PRO:CD    | 2.68                     | 0.41              |
| 2:c:46:ARG:HB2    | 2:c:84:LEU:HD12   | 2.01                     | 0.41              |
| 7:h:30:SER:HB2    | 7:h:81:LEU:HD13   | 2.01                     | 0.41              |
| 15:p:102:ARG:HH22 | 53:1:1754:A:C4'   | 2.23                     | 0.41              |
| 16:q:61:ILE:HG21  | 53:1:1010:A:H5'   | 2.02                     | 0.41              |
| 18:s:4:ILE:HG22   | 18:s:106:VAL:HG22 | 2.01                     | 0.41              |
| 20:u:10:VAL:HA    | 20:u:71:ILE:HA    | 2.01                     | 0.41              |
| 20:u:84:PHE:CB    | 53:1:297:G:H5''   | 2.44                     | 0.41              |
| 24:y:41:HIS:CD2   | 53:1:96:C:H4'     | 2.55                     | 0.41              |
| 28:D:34:ARG:HD3   | 53:1:467:G:OP2    | 2.20                     | 0.41              |
| 41:Q:49:ARG:NH2   | 52:3:522:C:H41    | 2.17                     | 0.41              |
| 47:W:59:LYS:H     | 47:W:59:LYS:HG2   | 1.68                     | 0.41              |
| 52:3:212:G:H2'    | 52:3:213:G:H8     | 1.85                     | 0.41              |
| 52:3:235:C:H2'    | 52:3:236:A:C8     | 2.55                     | 0.41              |
| 52:3:631:C:H5''   | 52:3:632:U:O4'    | 2.20                     | 0.41              |
| 52:3:1189:U:H2'   | 52:3:1190:G:H5'   | 2.01                     | 0.41              |
| 52:3:1305:G:H22   | 52:3:1331:G:H2'   | 1.84                     | 0.41              |
| 53:1:610:C:H2'    | 53:1:611:C:H6     | 1.85                     | 0.41              |
| 53:1:783:A:H2'    | 53:1:784:G:H5'    | 2.01                     | 0.41              |
| 53:1:2423:U:H5'   | 53:1:2424:C:C5'   | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:1:2443:C:H2'  | 53:1:2444:G:C8   | 2.56                     | 0.41              |
| 53:1:2547:A:H2'  | 53:1:2548:U:C6   | 2.54                     | 0.41              |
| 53:1:2689:U:O2   | 53:1:2713:U:H5'' | 2.21                     | 0.41              |
| 54:2:66:A:H5''   | 54:2:67:G:OP1    | 2.20                     | 0.41              |
| 1:b:128:THR:OG1  | 1:b:190:THR:HG22 | 2.20                     | 0.41              |
| 2:c:194:PRO:HA   | 53:1:2680:U:H5'  | 2.02                     | 0.41              |
| 4:e:153:ILE:HD12 | 4:e:153:ILE:N    | 2.35                     | 0.41              |
| 19:t:3:ARG:O     | 19:t:7:LEU:HD13  | 2.20                     | 0.41              |
| 25:z:23:LEU:HD21 | 25:z:53:MET:HE2  | 2.02                     | 0.41              |
| 32:H:190:THR:HB  | 32:H:193:GLY:O   | 2.19                     | 0.41              |
| 33:I:51:GLY:O    | 33:I:55:ARG:HG2  | 2.20                     | 0.41              |
| 45:U:46:LYS:NZ   | 45:U:48:GLU:HB3  | 2.35                     | 0.41              |
| 52:3:1412:C:H2'  | 52:3:1413:A:H8   | 1.84                     | 0.41              |
| 53:1:433:C:O2'   | 53:1:434:U:H5'   | 2.20                     | 0.41              |
| 53:1:2411:A:H2'  | 53:1:2412:A:C8   | 2.55                     | 0.41              |
| 53:1:2520:C:O2'  | 53:1:2521:C:H5'  | 2.19                     | 0.41              |
| 53:1:2809:A:H2'  | 53:1:2810:A:C8   | 2.55                     | 0.41              |
| 54:2:97:C:C2'    | 54:2:98:G:H5'    | 2.50                     | 0.41              |
| 56:4:17:U:O2'    | 56:4:18:G:H5'    | 2.21                     | 0.41              |
| 1:b:132:ARG:HB3  | 1:b:185:ALA:HB1  | 2.02                     | 0.41              |
| 1:b:180:MET:HB2  | 1:b:268:ARG:H    | 1.85                     | 0.41              |
| 2:c:133:THR:OG1  | 2:c:134:HIS:N    | 2.51                     | 0.41              |
| 6:g:57:LYS:HE3   | 6:g:57:LYS:HB3   | 1.96                     | 0.41              |
| 6:g:80:ILE:HB    | 6:g:146:VAL:HG22 | 2.01                     | 0.41              |
| 10:k:105:ARG:NH2 | 52:3:346:G:OP1   | 2.53                     | 0.41              |
| 15:p:13:LYS:HG2  | 15:p:76:HIS:ND1  | 2.36                     | 0.41              |
| 15:p:24:THR:HB   | 15:p:86:LYS:HB2  | 2.02                     | 0.41              |
| 31:G:153:MET:CE  | 31:G:157:PRO:HD3 | 2.50                     | 0.41              |
| 31:G:208:ALA:O   | 31:G:211:LEU:HG  | 2.21                     | 0.41              |
| 33:I:177:MET:N   | 33:I:177:MET:SD  | 2.94                     | 0.41              |
| 40:P:33:ILE:HG13 | 40:P:69:CYS:SG   | 2.61                     | 0.41              |
| 41:Q:88:ASP:C    | 41:Q:89:LEU:HD12 | 2.44                     | 0.41              |
| 41:Q:114:SER:N   | 52:3:502:A:OP1   | 2.53                     | 0.41              |
| 52:3:76:G:H2'    | 52:3:77:A:O4'    | 2.20                     | 0.41              |
| 52:3:756:C:H2'   | 52:3:757:U:O4'   | 2.19                     | 0.41              |
| 52:3:1230:C:H2'  | 52:3:1231:G:C8   | 2.55                     | 0.41              |
| 52:3:1245:C:H2'  | 52:3:1246:A:C8   | 2.56                     | 0.41              |
| 53:1:706:A:H2'   | 53:1:707:G:O4'   | 2.20                     | 0.41              |
| 53:1:898:C:H2'   | 53:1:899:A:O4'   | 2.20                     | 0.41              |
| 53:1:905:A:O2'   | 53:1:906:U:H5'   | 2.20                     | 0.41              |
| 53:1:1881:C:H2'  | 53:1:1882:U:O4'  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:1:2417:C:H2'  | 53:1:2418:A:C8   | 2.56                     | 0.41              |
| 53:1:2789:C:H2'  | 53:1:2790:U:H5'  | 2.01                     | 0.41              |
| 54:2:118:C:H2'   | 54:2:119:A:C8    | 2.55                     | 0.41              |
| 4:e:35:LEU:HB2   | 4:e:88:VAL:HG22  | 2.01                     | 0.41              |
| 43:S:26:LEU:O    | 43:S:30:ILE:HB   | 2.21                     | 0.41              |
| 52:3:59:A:H3'    | 52:3:331:G:H22   | 1.86                     | 0.41              |
| 52:3:1070:U:H2'  | 52:3:1071:C:C6   | 2.56                     | 0.41              |
| 53:1:242:G:N2    | 53:1:254:G:H2'   | 2.35                     | 0.41              |
| 53:1:479:A:H1'   | 53:1:481:G:H5''  | 2.02                     | 0.41              |
| 53:1:610:C:H2'   | 53:1:611:C:C6    | 2.55                     | 0.41              |
| 53:1:631:A:H2'   | 53:1:632:A:O4'   | 2.21                     | 0.41              |
| 53:1:690:G:O2'   | 53:1:691:C:H5'   | 2.20                     | 0.41              |
| 53:1:974:G:H1'   | 53:1:975:A:C8    | 2.55                     | 0.41              |
| 4:e:72:SER:HB2   | 4:e:80:GLN:HB2   | 2.02                     | 0.41              |
| 6:g:55:GLU:HA    | 6:g:58:LEU:HD12  | 2.02                     | 0.41              |
| 9:j:117:ALA:HA   | 9:j:120:ARG:HH21 | 1.85                     | 0.41              |
| 13:n:95:THR:OG1  | 13:n:96:ARG:N    | 2.53                     | 0.41              |
| 32:H:129:PHE:O   | 32:H:133:MET:HB3 | 2.21                     | 0.41              |
| 36:L:118:ARG:O   | 36:L:122:GLU:HG2 | 2.20                     | 0.41              |
| 39:O:5:ARG:HE    | 39:O:79:PRO:HD3  | 1.84                     | 0.41              |
| 42:R:68:LEU:HD23 | 42:R:71:GLU:OE1  | 2.21                     | 0.41              |
| 46:V:30:HIS:HA   | 46:V:31:PRO:HD3  | 1.90                     | 0.41              |
| 49:Y:83:ASN:HA   | 49:Y:86:ALA:OXT  | 2.21                     | 0.41              |
| 52:3:322:C:H2'   | 52:3:323:U:C6    | 2.56                     | 0.41              |
| 52:3:1137:C:H4'  | 52:3:1138:G:N2   | 2.36                     | 0.41              |
| 52:3:1288:A:H1'  | 52:3:1353:G:H4'  | 2.03                     | 0.41              |
| 53:1:2066:C:O2'  | 53:1:2067:G:H5'  | 2.20                     | 0.41              |
| 53:1:2511:U:H2'  | 53:1:2512:C:C6   | 2.55                     | 0.41              |
| 53:1:2545:G:C2'  | 53:1:2546:U:H5'  | 2.51                     | 0.41              |
| 2:c:125:TRP:CE3  | 2:c:160:LYS:HD3  | 2.55                     | 0.41              |
| 10:k:15:GLY:O    | 10:k:47:ILE:HG12 | 2.20                     | 0.41              |
| 10:k:61:VAL:O    | 10:k:61:VAL:HG13 | 2.20                     | 0.41              |
| 34:J:92:ARG:O    | 34:J:93:VAL:C    | 2.62                     | 0.41              |
| 36:L:8:GLN:NE2   | 36:L:9:ARG:HG2   | 2.36                     | 0.41              |
| 51:a:50:ILE:HG22 | 51:a:204:ALA:HB2 | 2.02                     | 0.41              |
| 52:3:156:C:H2'   | 52:3:157:U:O4'   | 2.20                     | 0.41              |
| 52:3:205:A:H2'   | 52:3:206:C:O4'   | 2.21                     | 0.41              |
| 52:3:1346:A:H2'  | 52:3:1346:A:N3   | 2.36                     | 0.41              |
| 53:1:129:C:H2'   | 53:1:130:C:C6    | 2.56                     | 0.41              |
| 53:1:1258:U:H2'  | 53:1:1259:G:H8   | 1.84                     | 0.41              |
| 53:1:1570:A:H2'  | 53:1:1571:A:C8   | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:1889:A:H2'   | 53:1:1890:A:C8    | 2.56                     | 0.41              |
| 53:1:2071:A:H2'   | 53:1:2072:C:C6    | 2.56                     | 0.41              |
| 53:1:2313:C:H2'   | 53:1:2314:A:H8    | 1.85                     | 0.41              |
| 53:1:2345:G:H5'   | 53:1:2347:C:H5'   | 2.01                     | 0.41              |
| 54:2:114:C:H2'    | 54:2:115:A:H8     | 1.85                     | 0.41              |
| 55:5:38:A:H2'     | 55:5:39:C:O4'     | 2.20                     | 0.41              |
| 1:b:252:LYS:NZ    | 53:1:1901:A:H4'   | 2.35                     | 0.41              |
| 10:k:69:VAL:O     | 10:k:76:VAL:HA    | 2.21                     | 0.41              |
| 16:q:75:TYR:HE2   | 53:1:1153:C:H5'   | 1.85                     | 0.41              |
| 17:r:51:VAL:HG22  | 17:r:52:PRO:CD    | 2.50                     | 0.41              |
| 18:s:28:LYS:HZ2   | 18:s:68:ASP:HA    | 1.85                     | 0.41              |
| 23:x:24:THR:HG21  | 53:1:2081:U:H4'   | 2.02                     | 0.41              |
| 27:C:50:GLU:HG3   | 27:C:51:ALA:N     | 2.35                     | 0.41              |
| 33:I:96:ARG:O     | 33:I:100:VAL:HG23 | 2.21                     | 0.41              |
| 41:Q:49:ARG:NE    | 41:Q:88:ASP:OD2   | 2.53                     | 0.41              |
| 52:3:948:C:H2'    | 52:3:949:A:C8     | 2.55                     | 0.41              |
| 52:3:1323:G:H2'   | 52:3:1324:A:C8    | 2.56                     | 0.41              |
| 52:3:1347:G:O2'   | 52:3:1348:U:H5    | 2.04                     | 0.41              |
| 53:1:371:A:N6     | 53:1:401:A:H3'    | 2.35                     | 0.41              |
| 53:1:817:C:O2'    | 53:1:839:U:H5''   | 2.20                     | 0.41              |
| 53:1:833:A:H2'    | 53:1:834:G:H8     | 1.86                     | 0.41              |
| 53:1:1709:U:H2'   | 53:1:1710:G:H8    | 1.85                     | 0.41              |
| 53:1:2121:G:H2'   | 53:1:2122:U:O4'   | 2.20                     | 0.41              |
| 53:1:2200:C:H2'   | 53:1:2201:G:C8    | 2.55                     | 0.41              |
| 53:1:2583:G:H2'   | 53:1:2584:U:O4'   | 2.21                     | 0.41              |
| 1:b:48:ILE:HG23   | 1:b:48:ILE:O      | 2.20                     | 0.41              |
| 1:b:107:LYS:HE2   | 1:b:195:GLY:HA2   | 2.03                     | 0.41              |
| 1:b:224:MET:HE2   | 53:1:782:A:N1     | 2.35                     | 0.41              |
| 1:b:241:LYS:O     | 53:1:1902:C:H4'   | 2.20                     | 0.41              |
| 3:d:148:ILE:HB    | 3:d:169:VAL:HG12  | 2.03                     | 0.41              |
| 6:g:77:THR:HG23   | 6:g:143:ILE:HG23  | 2.03                     | 0.41              |
| 6:g:110:VAL:HG22  | 6:g:111:ALA:N     | 2.36                     | 0.41              |
| 9:j:18:VAL:HG12   | 9:j:140:LEU:HB3   | 2.02                     | 0.41              |
| 9:j:128:ASN:HB2   | 9:j:129:GLU:OE2   | 2.21                     | 0.41              |
| 18:s:29:VAL:HG21  | 18:s:69:LEU:HB3   | 2.03                     | 0.41              |
| 21:v:82:TYR:CZ    | 21:v:83:LYS:HE3   | 2.55                     | 0.41              |
| 31:G:147:LEU:HD23 | 31:G:150:ILE:HD11 | 2.03                     | 0.41              |
| 32:H:39:ARG:NH1   | 32:H:54:ILE:HG13  | 2.35                     | 0.41              |
| 33:I:112:GLU:HG2  | 52:3:407:U:O2'    | 2.21                     | 0.41              |
| 34:J:88:HIS:O     | 34:J:89:THR:HG22  | 2.20                     | 0.41              |
| 35:K:18:VAL:CG1   | 35:K:19:PRO:HD3   | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 35:K:73:GLU:O    | 35:K:77:THR:HG23 | 2.21                     | 0.41              |
| 36:L:78:ARG:CZ   | 52:3:1382:C:H4'  | 2.51                     | 0.41              |
| 40:P:28:ASN:HB2  | 52:3:690:G:OP2   | 2.20                     | 0.41              |
| 40:P:72:ALA:N    | 40:P:74:LYS:HZ1  | 2.17                     | 0.41              |
| 43:S:30:ILE:HG22 | 43:S:30:ILE:O    | 2.21                     | 0.41              |
| 43:S:34:ASN:CG   | 43:S:35:ALA:H    | 2.28                     | 0.41              |
| 43:S:74:ARG:NH2  | 52:3:1359:C:H3'  | 2.35                     | 0.41              |
| 44:T:86:LEU:HB3  | 44:T:87:ARG:H    | 1.56                     | 0.41              |
| 51:a:8:MET:HA    | 51:a:11:ILE:HD12 | 2.03                     | 0.41              |
| 52:3:103:U:H2'   | 52:3:104:G:O4'   | 2.21                     | 0.41              |
| 52:3:390:U:H2'   | 52:3:391:G:H8    | 1.86                     | 0.41              |
| 52:3:600:A:H2'   | 52:3:601:G:C8    | 2.55                     | 0.41              |
| 52:3:1411:C:H2'  | 52:3:1412:C:C6   | 2.56                     | 0.41              |
| 53:1:319:G:H2'   | 53:1:320:A:O4'   | 2.20                     | 0.41              |
| 53:1:796:C:H2'   | 53:1:797:G:C8    | 2.55                     | 0.41              |
| 53:1:864:G:O2'   | 53:1:865:C:H5'   | 2.20                     | 0.41              |
| 53:1:1373:A:C5'  | 53:1:2212:A:H1'  | 2.50                     | 0.41              |
| 53:1:1885:A:H2'  | 53:1:1886:U:H5'  | 2.02                     | 0.41              |
| 53:1:2515:C:H2'  | 53:1:2516:A:C8   | 2.56                     | 0.41              |
| 55:5:18:G:H1     | 55:5:55:U:H6     | 1.68                     | 0.41              |
| 55:5:51:C:H2'    | 55:5:52:G:C8     | 2.56                     | 0.41              |
| 57:7:17:C:O5'    | 57:7:18:G:H5''   | 2.21                     | 0.41              |
| 11:l:38:GLN:HG3  | 53:1:805:G:H5''  | 2.03                     | 0.41              |
| 18:s:74:ILE:O    | 18:s:74:ILE:HG23 | 2.21                     | 0.41              |
| 18:s:83:LYS:O    | 18:s:84:ARG:NH2  | 2.54                     | 0.41              |
| 24:y:21:LEU:O    | 24:y:25:GLN:HB3  | 2.21                     | 0.41              |
| 39:O:68:ARG:HB3  | 39:O:70:HIS:CE1  | 2.55                     | 0.41              |
| 44:T:66:LEU:HD12 | 44:T:87:ARG:HH21 | 1.86                     | 0.41              |
| 52:3:662:U:H2'   | 52:3:663:A:C8    | 2.56                     | 0.41              |
| 52:3:911:U:H2'   | 52:3:912:C:C6    | 2.55                     | 0.41              |
| 53:1:573:U:O4    | 53:1:2030:A:H3'  | 2.21                     | 0.41              |
| 53:1:1251:C:O2'  | 53:1:1252:G:H3'  | 2.21                     | 0.41              |
| 53:1:1421:G:H1'  | 53:1:1494:A:N6   | 2.36                     | 0.41              |
| 53:1:1877:A:H2'  | 53:1:1878:G:O4'  | 2.21                     | 0.41              |
| 53:1:1931:U:O2   | 53:1:1931:U:H2'  | 2.20                     | 0.41              |
| 53:1:2039:U:H2'  | 53:1:2040:G:H8   | 1.85                     | 0.41              |
| 1:b:52:HIS:HD2   | 53:1:1824:G:OP2  | 2.04                     | 0.40              |
| 3:d:131:THR:HG23 | 53:1:321:U:H5''  | 2.02                     | 0.40              |
| 9:j:11:VAL:HG23  | 9:j:50:THR:HG23  | 2.03                     | 0.40              |
| 13:n:12:ARG:O    | 53:1:2002:G:H5'  | 2.21                     | 0.40              |
| 16:q:24:TYR:CE1  | 53:1:17:G:H4'    | 2.57                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:E:6:VAL:HG13  | 29:E:6:VAL:O      | 2.21                     | 0.40              |
| 35:K:18:VAL:HG12 | 35:K:19:PRO:HD3   | 2.01                     | 0.40              |
| 35:K:45:ARG:C    | 35:K:56:LYS:HD3   | 2.45                     | 0.40              |
| 40:P:32:THR:HG23 | 40:P:43:TRP:HB3   | 2.03                     | 0.40              |
| 40:P:51:PHE:HE2  | 40:P:64:VAL:HG11  | 1.85                     | 0.40              |
| 50:Z:19:LYS:HB3  | 50:Z:24:LYS:HD2   | 2.04                     | 0.40              |
| 52:3:1453:G:N3   | 52:3:1453:G:H3'   | 2.36                     | 0.40              |
| 53:1:406:G:H2'   | 53:1:407:G:H8     | 1.86                     | 0.40              |
| 53:1:538:A:H2'   | 53:1:539:G:O4'    | 2.19                     | 0.40              |
| 54:2:22:U:H2'    | 54:2:23:G:C8      | 2.56                     | 0.40              |
| 5:f:86:LEU:HD12  | 5:f:86:LEU:N      | 2.37                     | 0.40              |
| 10:k:43:ILE:HD12 | 10:k:56:ASP:HB2   | 2.03                     | 0.40              |
| 13:n:79:LEU:O    | 13:n:80:PHE:HB2   | 2.20                     | 0.40              |
| 26:B:30:ASP:HB3  | 26:B:34:GLY:N     | 2.36                     | 0.40              |
| 32:H:76:ILE:HD11 | 32:H:102:ILE:HD13 | 2.03                     | 0.40              |
| 35:K:49:TYR:OH   | 35:K:86:ARG:NH1   | 2.54                     | 0.40              |
| 36:L:70:PRO:HG3  | 36:L:98:LEU:HD22  | 2.03                     | 0.40              |
| 39:O:8:ILE:HD12  | 39:O:8:ILE:N      | 2.37                     | 0.40              |
| 40:P:22:ILE:HG23 | 40:P:22:ILE:O     | 2.21                     | 0.40              |
| 40:P:22:ILE:HG12 | 40:P:95:THR:HG21  | 2.04                     | 0.40              |
| 41:Q:49:ARG:HH21 | 52:3:522:C:H41    | 1.69                     | 0.40              |
| 44:T:71:ARG:NH2  | 52:3:754:C:H5'    | 2.36                     | 0.40              |
| 52:3:423:G:H2'   | 52:3:424:G:H5'    | 2.03                     | 0.40              |
| 52:3:742:G:H2'   | 52:3:743:A:C8     | 2.56                     | 0.40              |
| 52:3:777:A:H2'   | 52:3:778:G:O4'    | 2.22                     | 0.40              |
| 53:1:163:C:H2'   | 53:1:164:C:O4'    | 2.21                     | 0.40              |
| 53:1:1015:U:H2'  | 53:1:1016:G:C8    | 2.55                     | 0.40              |
| 53:1:2087:G:H2'  | 53:1:2088:A:C8    | 2.57                     | 0.40              |
| 53:1:2368:C:H2'  | 53:1:2369:A:H8    | 1.86                     | 0.40              |
| 55:5:11:A:H2'    | 55:5:12:G:H8      | 1.86                     | 0.40              |
| 55:6:41:C:H2'    | 55:6:42:G:C8      | 2.56                     | 0.40              |
| 1:b:225:ASN:ND2  | 53:1:784:G:O4'    | 2.54                     | 0.40              |
| 6:g:97:ARG:HD3   | 6:g:97:ARG:HA     | 1.93                     | 0.40              |
| 11:l:42:SER:HB2  | 53:1:672:C:H5     | 1.87                     | 0.40              |
| 12:m:26:VAL:HG23 | 12:m:104:GLU:OE1  | 2.22                     | 0.40              |
| 14:o:85:LYS:HA   | 14:o:85:LYS:HD3   | 1.86                     | 0.40              |
| 38:N:6:TYR:CG    | 38:N:7:GLY:N      | 2.89                     | 0.40              |
| 38:N:30:ASN:O    | 38:N:31:GLN:HB2   | 2.22                     | 0.40              |
| 39:O:29:ALA:O    | 39:O:33:GLY:CA    | 2.69                     | 0.40              |
| 41:Q:33:CYS:HA   | 41:Q:54:VAL:HA    | 2.02                     | 0.40              |
| 50:Z:57:LYS:HG3  | 50:Z:61:ARG:HG3   | 2.03                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 52:3:41:G:H2'    | 52:3:42:G:H8      | 1.87                     | 0.40              |
| 52:3:244:U:O4    | 52:3:906:A:H1'    | 2.22                     | 0.40              |
| 52:3:715:A:H5''  | 52:3:805:C:H1'    | 2.04                     | 0.40              |
| 52:3:1238:A:C2'  | 52:3:1239:A:H5'   | 2.50                     | 0.40              |
| 53:1:118:A:OP2   | 53:1:119:A:H2'    | 2.22                     | 0.40              |
| 53:1:558:U:H2'   | 53:1:559:G:H8     | 1.87                     | 0.40              |
| 53:1:1535:A:H3'  | 53:1:1536:C:H5'   | 2.03                     | 0.40              |
| 53:1:1610:A:H3'  | 53:1:1611:C:H5'   | 2.03                     | 0.40              |
| 53:1:2498:C:O2'  | 53:1:2499:C:H5'   | 2.22                     | 0.40              |
| 1:b:32:LEU:C     | 1:b:33:LEU:HD12   | 2.46                     | 0.40              |
| 1:b:70:LYS:O     | 1:b:117:SER:OG    | 2.40                     | 0.40              |
| 1:b:228:ASP:CG   | 53:1:780:G:H1     | 2.29                     | 0.40              |
| 4:e:105:ILE:HD12 | 4:e:138:PRO:HG2   | 2.02                     | 0.40              |
| 8:i:126:ARG:HG3  | 53:1:1080:A:O2'   | 2.21                     | 0.40              |
| 11:l:30:THR:HG22 | 53:1:810:U:O4     | 2.21                     | 0.40              |
| 18:s:1:MET:SD    | 18:s:62:ASP:HB3   | 2.62                     | 0.40              |
| 25:z:50:VAL:O    | 25:z:54:VAL:HG12  | 2.20                     | 0.40              |
| 36:L:68:VAL:HG23 | 36:L:99:ALA:HB1   | 2.03                     | 0.40              |
| 37:M:34:ALA:HB1  | 37:M:109:VAL:HG11 | 2.03                     | 0.40              |
| 51:a:23:ILE:HG13 | 51:a:189:LEU:HD12 | 2.03                     | 0.40              |
| 52:3:346:G:H2'   | 52:3:347:G:H5'    | 2.04                     | 0.40              |
| 52:3:381:C:H2'   | 52:3:382:A:O4'    | 2.21                     | 0.40              |
| 52:3:890:G:O2'   | 52:3:891:U:C5     | 2.75                     | 0.40              |
| 52:3:918:A:H2'   | 52:3:919:A:O4'    | 2.21                     | 0.40              |
| 52:3:1175:G:H2'  | 52:3:1176:A:C8    | 2.56                     | 0.40              |
| 53:1:279:A:C2'   | 53:1:280:U:H5'    | 2.51                     | 0.40              |
| 53:1:414:C:H2'   | 53:1:415:A:H8     | 1.85                     | 0.40              |
| 53:1:511:U:C2'   | 53:1:512:G:H5'    | 2.50                     | 0.40              |
| 53:1:1278:C:H2'  | 53:1:1279:G:H8    | 1.86                     | 0.40              |
| 53:1:1971:U:H5'  | 53:1:1972:G:H5''  | 2.03                     | 0.40              |
| 53:1:2327:A:H2'  | 53:1:2328:A:C8    | 2.56                     | 0.40              |
| 53:1:2345:G:H4'  | 53:1:2346:A:H3'   | 2.03                     | 0.40              |
| 1:b:164:VAL:HG13 | 52:3:712:A:H5''   | 2.02                     | 0.40              |
| 3:d:5:LEU:HD13   | 3:d:10:SER:O      | 2.22                     | 0.40              |
| 8:i:24:GLY:HA3   | 8:i:25:PRO:HD3    | 1.82                     | 0.40              |
| 11:l:55:MET:HA   | 11:l:56:PRO:HD3   | 1.90                     | 0.40              |
| 19:t:73:ARG:HD3  | 19:t:73:ARG:N     | 2.37                     | 0.40              |
| 35:K:11:HIS:HA   | 35:K:12:PRO:HD3   | 1.99                     | 0.40              |
| 36:L:1:PRO:HD3   | 52:3:1377:A:N3    | 2.37                     | 0.40              |
| 36:L:55:LYS:HB2  | 36:L:60:ALA:HB2   | 2.03                     | 0.40              |
| 36:L:109:LYS:HG3 | 36:L:110:ARG:H    | 1.86                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 38:N:79:ARG:HD2 | 38:N:102:PHE:CE1 | 2.57                     | 0.40              |
| 39:O:12:ALA:HB3 | 39:O:18:ILE:CG2  | 2.51                     | 0.40              |
| 43:S:41:TRP:O   | 43:S:45:LEU:HD13 | 2.20                     | 0.40              |
| 52:3:103:U:H5'  | 52:3:151:A:H1'   | 2.03                     | 0.40              |
| 52:3:396:C:C3'  | 52:3:397:A:H5''  | 2.51                     | 0.40              |
| 52:3:767:A:H2'  | 52:3:768:A:O4'   | 2.22                     | 0.40              |
| 52:3:1497:G:C2' | 52:3:1498:U:H5'  | 2.51                     | 0.40              |
| 53:1:254:G:C2'  | 53:1:255:A:H5''  | 2.51                     | 0.40              |
| 53:1:546:U:H2'  | 53:1:547:A:C4'   | 2.51                     | 0.40              |
| 53:1:815:C:H2'  | 53:1:816:C:C6    | 2.55                     | 0.40              |
| 53:1:1042:G:H2' | 53:1:1043:C:O4'  | 2.21                     | 0.40              |
| 53:1:2011:U:H2' | 53:1:2012:G:O4'  | 2.21                     | 0.40              |
| 53:1:2243:U:H2' | 53:1:2244:U:C6   | 2.56                     | 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%) | 240 (89%) | 24 (9%)  | 5 (2%)   | 6           | 33  |
| 2   | c     | 207/209 (99%) | 181 (87%) | 26 (13%) | 0        | 100         | 100 |
| 3   | d     | 199/201 (99%) | 185 (93%) | 13 (6%)  | 1 (0%)   | 24          | 57  |
| 4   | e     | 175/177 (99%) | 152 (87%) | 22 (13%) | 1 (1%)   | 21          | 54  |
| 5   | f     | 174/176 (99%) | 163 (94%) | 9 (5%)   | 2 (1%)   | 11          | 43  |
| 6   | g     | 147/149 (99%) | 129 (88%) | 16 (11%) | 2 (1%)   | 9           | 38  |
| 7   | h     | 129/131 (98%) | 98 (76%)  | 26 (20%) | 5 (4%)   | 2           | 20  |
| 8   | i     | 139/141 (99%) | 120 (86%) | 18 (13%) | 1 (1%)   | 18          | 51  |
| 9   | j     | 140/142 (99%) | 130 (93%) | 9 (6%)   | 1 (1%)   | 18          | 51  |
| 10  | k     | 120/122 (98%) | 97 (81%)  | 19 (16%) | 4 (3%)   | 3           | 24  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 11  | l     | 141/143 (99%) | 116 (82%) | 22 (16%) | 3 (2%)   | 5           | 31  |
| 12  | m     | 134/136 (98%) | 123 (92%) | 8 (6%)   | 3 (2%)   | 5           | 30  |
| 13  | n     | 118/120 (98%) | 97 (82%)  | 20 (17%) | 1 (1%)   | 16          | 49  |
| 14  | o     | 114/116 (98%) | 103 (90%) | 9 (8%)   | 2 (2%)   | 6           | 34  |
| 15  | p     | 112/114 (98%) | 97 (87%)  | 14 (12%) | 1 (1%)   | 14          | 46  |
| 16  | q     | 115/117 (98%) | 106 (92%) | 8 (7%)   | 1 (1%)   | 14          | 46  |
| 17  | r     | 101/103 (98%) | 83 (82%)  | 14 (14%) | 4 (4%)   | 2           | 20  |
| 18  | s     | 108/110 (98%) | 99 (92%)  | 7 (6%)   | 2 (2%)   | 6           | 33  |
| 19  | t     | 91/93 (98%)   | 81 (89%)  | 9 (10%)  | 1 (1%)   | 11          | 43  |
| 20  | u     | 100/102 (98%) | 86 (86%)  | 10 (10%) | 4 (4%)   | 2           | 20  |
| 21  | v     | 92/94 (98%)   | 84 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 22  | w     | 73/75 (97%)   | 64 (88%)  | 9 (12%)  | 0        | 100         | 100 |
| 23  | x     | 75/77 (97%)   | 69 (92%)  | 5 (7%)   | 1 (1%)   | 9           | 39  |
| 24  | y     | 61/63 (97%)   | 54 (88%)  | 7 (12%)  | 0        | 100         | 100 |
| 25  | z     | 56/58 (97%)   | 52 (93%)  | 4 (7%)   | 0        | 100         | 100 |
| 26  | B     | 54/56 (96%)   | 49 (91%)  | 4 (7%)   | 1 (2%)   | 6           | 33  |
| 27  | C     | 48/50 (96%)   | 45 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 28  | D     | 44/46 (96%)   | 41 (93%)  | 1 (2%)   | 2 (4%)   | 2           | 17  |
| 29  | E     | 62/64 (97%)   | 53 (86%)  | 8 (13%)  | 1 (2%)   | 7           | 36  |
| 30  | F     | 36/38 (95%)   | 31 (86%)  | 4 (11%)  | 1 (3%)   | 4           | 26  |
| 31  | G     | 223/225 (99%) | 200 (90%) | 22 (10%) | 1 (0%)   | 30          | 61  |
| 32  | H     | 204/206 (99%) | 189 (93%) | 15 (7%)  | 0        | 100         | 100 |
| 33  | I     | 203/205 (99%) | 176 (87%) | 23 (11%) | 4 (2%)   | 6           | 32  |
| 34  | J     | 155/157 (99%) | 126 (81%) | 22 (14%) | 7 (4%)   | 2           | 17  |
| 35  | K     | 98/100 (98%)  | 76 (78%)  | 18 (18%) | 4 (4%)   | 2           | 19  |
| 36  | L     | 149/151 (99%) | 132 (89%) | 14 (9%)  | 3 (2%)   | 6           | 32  |
| 37  | M     | 127/129 (98%) | 111 (87%) | 15 (12%) | 1 (1%)   | 16          | 49  |
| 38  | N     | 125/127 (98%) | 101 (81%) | 18 (14%) | 6 (5%)   | 2           | 16  |
| 39  | O     | 96/98 (98%)   | 77 (80%)  | 14 (15%) | 5 (5%)   | 1           | 15  |
| 40  | P     | 114/116 (98%) | 95 (83%)  | 14 (12%) | 5 (4%)   | 2           | 18  |
| 41  | Q     | 121/123 (98%) | 95 (78%)  | 20 (16%) | 6 (5%)   | 1           | 16  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 42  | R     | 112/114 (98%)   | 96 (86%)   | 12 (11%)  | 4 (4%)   | 2           | 22  |
| 43  | S     | 98/100 (98%)    | 85 (87%)   | 12 (12%)  | 1 (1%)   | 12          | 45  |
| 44  | T     | 86/88 (98%)     | 75 (87%)   | 10 (12%)  | 1 (1%)   | 10          | 41  |
| 45  | U     | 80/82 (98%)     | 70 (88%)   | 9 (11%)   | 1 (1%)   | 9           | 39  |
| 46  | V     | 78/80 (98%)     | 62 (80%)   | 14 (18%)  | 2 (3%)   | 4           | 27  |
| 47  | W     | 63/65 (97%)     | 57 (90%)   | 5 (8%)    | 1 (2%)   | 7           | 36  |
| 48  | X     | 77/79 (98%)     | 66 (86%)   | 10 (13%)  | 1 (1%)   | 9           | 39  |
| 49  | Y     | 83/85 (98%)     | 79 (95%)   | 3 (4%)    | 1 (1%)   | 10          | 41  |
| 50  | Z     | 63/65 (97%)     | 40 (64%)   | 19 (30%)  | 4 (6%)   | 1           | 12  |
| 51  | a     | 130/223 (58%)   | 126 (97%)  | 4 (3%)    | 0        | 100         | 100 |
| All | All   | 5919/6112 (97%) | 5162 (87%) | 649 (11%) | 108 (2%) | 9           | 34  |

All (108) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | d     | 83  | VAL  |
| 7   | h     | 108 | VAL  |
| 7   | h     | 118 | ILE  |
| 11  | l     | 31  | GLY  |
| 11  | l     | 85  | VAL  |
| 20  | u     | 51  | LEU  |
| 26  | B     | 23  | ALA  |
| 29  | E     | 31  | ILE  |
| 30  | F     | 37  | GLN  |
| 34  | J     | 89  | THR  |
| 34  | J     | 93  | VAL  |
| 34  | J     | 98  | ALA  |
| 34  | J     | 122 | VAL  |
| 35  | K     | 53  | LYS  |
| 35  | K     | 54  | LEU  |
| 35  | K     | 92  | THR  |
| 36  | L     | 56  | SER  |
| 38  | N     | 57  | VAL  |
| 38  | N     | 90  | ASP  |
| 38  | N     | 91  | GLU  |
| 39  | O     | 37  | ARG  |
| 40  | P     | 13  | LYS  |
| 40  | P     | 125 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | Q     | 24  | GLU  |
| 46  | V     | 49  | ASN  |
| 49  | Y     | 68  | LYS  |
| 1   | b     | 240 | GLY  |
| 5   | f     | 174 | LYS  |
| 5   | f     | 175 | LYS  |
| 6   | g     | 41  | LYS  |
| 10  | k     | 35  | VAL  |
| 10  | k     | 92  | GLU  |
| 12  | m     | 58  | LYS  |
| 15  | p     | 113 | LEU  |
| 17  | r     | 53  | PHE  |
| 18  | s     | 63  | GLY  |
| 20  | u     | 56  | GLY  |
| 28  | D     | 4   | THR  |
| 34  | J     | 11  | GLN  |
| 36  | L     | 18  | GLY  |
| 38  | N     | 8   | THR  |
| 39  | O     | 58  | ASN  |
| 40  | P     | 89  | GLY  |
| 41  | Q     | 28  | GLN  |
| 42  | R     | 6   | ILE  |
| 42  | R     | 65  | GLU  |
| 45  | U     | 79  | ASN  |
| 46  | V     | 17  | GLU  |
| 48  | X     | 4   | LEU  |
| 50  | Z     | 24  | LYS  |
| 1   | b     | 237 | ARG  |
| 1   | b     | 260 | LYS  |
| 4   | e     | 175 | PRO  |
| 11  | l     | 29  | LYS  |
| 18  | s     | 3   | THR  |
| 20  | u     | 97  | SER  |
| 28  | D     | 5   | PHE  |
| 31  | G     | 154 | GLY  |
| 34  | J     | 90  | GLY  |
| 35  | K     | 86  | ARG  |
| 38  | N     | 12  | LYS  |
| 42  | R     | 4   | ALA  |
| 42  | R     | 14  | ALA  |
| 43  | S     | 3   | GLN  |
| 47  | W     | 13  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | Z     | 9   | GLU  |
| 7   | h     | 81  | LEU  |
| 10  | k     | 72  | PRO  |
| 10  | k     | 93  | GLN  |
| 12  | m     | 6   | ARG  |
| 16  | q     | 27  | ARG  |
| 19  | t     | 72  | GLN  |
| 33  | I     | 4   | LEU  |
| 33  | I     | 19  | PHE  |
| 33  | I     | 47  | LEU  |
| 34  | J     | 121 | ASN  |
| 37  | M     | 47  | ASP  |
| 38  | N     | 100 | ALA  |
| 39  | O     | 89  | ARG  |
| 40  | P     | 88  | PRO  |
| 41  | Q     | 33  | CYS  |
| 41  | Q     | 35  | ARG  |
| 41  | Q     | 77  | SER  |
| 41  | Q     | 122 | LYS  |
| 44  | T     | 46  | LYS  |
| 50  | Z     | 64  | ALA  |
| 1   | b     | 154 | ALA  |
| 13  | n     | 104 | ALA  |
| 14  | o     | 100 | HIS  |
| 17  | r     | 52  | PRO  |
| 17  | r     | 55  | ASP  |
| 39  | O     | 42  | LEU  |
| 39  | O     | 75  | ASP  |
| 40  | P     | 92  | ARG  |
| 14  | o     | 34  | HIS  |
| 17  | r     | 54  | VAL  |
| 20  | u     | 54  | PRO  |
| 23  | x     | 11  | PRO  |
| 33  | I     | 167 | PRO  |
| 50  | Z     | 34  | ARG  |
| 1   | b     | 205 | GLY  |
| 6   | g     | 3   | VAL  |
| 7   | h     | 77  | VAL  |
| 7   | h     | 90  | GLY  |
| 8   | i     | 92  | PRO  |
| 9   | j     | 81  | ILE  |
| 12  | m     | 15  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | L     | 15  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | b     | 216/216 (100%) | 216 (100%) | 0        | 100         | 100 |
| 2   | c     | 164/164 (100%) | 164 (100%) | 0        | 100         | 100 |
| 3   | d     | 165/165 (100%) | 165 (100%) | 0        | 100         | 100 |
| 4   | e     | 148/148 (100%) | 148 (100%) | 0        | 100         | 100 |
| 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%) | 98 (98%)   | 2 (2%)   | 48          | 66  |
| 8   | i     | 109/109 (100%) | 108 (99%)  | 1 (1%)   | 70          | 76  |
| 9   | j     | 116/116 (100%) | 116 (100%) | 0        | 100         | 100 |
| 10  | k     | 103/103 (100%) | 102 (99%)  | 1 (1%)   | 68          | 75  |
| 11  | l     | 102/102 (100%) | 101 (99%)  | 1 (1%)   | 68          | 75  |
| 12  | m     | 109/109 (100%) | 108 (99%)  | 1 (1%)   | 70          | 76  |
| 13  | n     | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 14  | o     | 86/86 (100%)   | 84 (98%)   | 2 (2%)   | 44          | 64  |
| 15  | p     | 99/99 (100%)   | 97 (98%)   | 2 (2%)   | 48          | 66  |
| 16  | q     | 89/89 (100%)   | 88 (99%)   | 1 (1%)   | 65          | 74  |
| 17  | r     | 84/84 (100%)   | 84 (100%)  | 0        | 100         | 100 |
| 18  | s     | 93/93 (100%)   | 93 (100%)  | 0        | 100         | 100 |
| 19  | t     | 80/80 (100%)   | 80 (100%)  | 0        | 100         | 100 |
| 20  | u     | 83/83 (100%)   | 83 (100%)  | 0        | 100         | 100 |
| 21  | v     | 78/78 (100%)   | 78 (100%)  | 0        | 100         | 100 |
| 22  | w     | 57/57 (100%)   | 57 (100%)  | 0        | 100         | 100 |
| 23  | x     | 67/67 (100%)   | 67 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 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%)    | 45 (100%)   | 0        | 100         | 100 |
| 28  | D     | 38/38 (100%)    | 38 (100%)   | 0        | 100         | 100 |
| 29  | E     | 51/51 (100%)    | 51 (100%)   | 0        | 100         | 100 |
| 30  | F     | 34/34 (100%)    | 33 (97%)    | 1 (3%)   | 37          | 60  |
| 31  | G     | 186/186 (100%)  | 185 (100%)  | 1 (0%)   | 81          | 80  |
| 32  | H     | 170/170 (100%)  | 169 (99%)   | 1 (1%)   | 78          | 79  |
| 33  | I     | 172/172 (100%)  | 172 (100%)  | 0        | 100         | 100 |
| 34  | J     | 119/119 (100%)  | 118 (99%)   | 1 (1%)   | 73          | 77  |
| 35  | K     | 87/87 (100%)    | 86 (99%)    | 1 (1%)   | 65          | 74  |
| 36  | L     | 124/124 (100%)  | 124 (100%)  | 0        | 100         | 100 |
| 37  | M     | 104/104 (100%)  | 103 (99%)   | 1 (1%)   | 68          | 75  |
| 38  | N     | 105/105 (100%)  | 105 (100%)  | 0        | 100         | 100 |
| 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%)  | 102 (99%)   | 1 (1%)   | 68          | 75  |
| 42  | R     | 92/92 (100%)    | 92 (100%)   | 0        | 100         | 100 |
| 43  | S     | 83/83 (100%)    | 82 (99%)    | 1 (1%)   | 63          | 73  |
| 44  | T     | 76/76 (100%)    | 76 (100%)   | 0        | 100         | 100 |
| 45  | U     | 65/65 (100%)    | 64 (98%)    | 1 (2%)   | 57          | 70  |
| 46  | V     | 74/74 (100%)    | 73 (99%)    | 1 (1%)   | 59          | 71  |
| 47  | W     | 56/56 (100%)    | 55 (98%)    | 1 (2%)   | 51          | 68  |
| 48  | X     | 70/70 (100%)    | 70 (100%)   | 0        | 100         | 100 |
| 49  | Y     | 65/65 (100%)    | 65 (100%)   | 0        | 100         | 100 |
| 50  | Z     | 55/55 (100%)    | 53 (96%)    | 2 (4%)   | 31          | 56  |
| 51  | a     | 110/174 (63%)   | 110 (100%)  | 0        | 100         | 100 |
| All | All   | 4908/4972 (99%) | 4883 (100%) | 25 (0%)  | 78          | 80  |

All (25) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | h     | 77  | VAL  |
| 7   | h     | 118 | ILE  |
| 8   | i     | 100 | ILE  |
| 10  | k     | 89  | ASN  |
| 11  | l     | 94  | THR  |
| 12  | m     | 26  | VAL  |
| 14  | o     | 31  | THR  |
| 14  | o     | 90  | VAL  |
| 15  | p     | 12  | MET  |
| 15  | p     | 83  | ILE  |
| 16  | q     | 30  | VAL  |
| 30  | F     | 26  | ILE  |
| 31  | G     | 67  | LEU  |
| 32  | H     | 156 | LEU  |
| 34  | J     | 105 | ILE  |
| 35  | K     | 54  | LEU  |
| 37  | M     | 75  | GLN  |
| 39  | O     | 89  | ARG  |
| 41  | Q     | 75  | GLU  |
| 43  | S     | 47  | LEU  |
| 45  | U     | 48  | GLU  |
| 46  | V     | 79  | GLU  |
| 47  | W     | 12  | PHE  |
| 50  | Z     | 23  | GLU  |
| 50  | Z     | 37  | TYR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 20  | ASN  |
| 1   | b     | 36  | ASN  |
| 1   | b     | 52  | HIS  |
| 1   | b     | 59  | GLN  |
| 1   | b     | 89  | ASN  |
| 1   | b     | 127 | ASN  |
| 1   | b     | 225 | ASN  |
| 1   | b     | 238 | ASN  |
| 2   | c     | 32  | ASN  |
| 2   | c     | 49  | GLN  |
| 2   | c     | 94  | GLN  |
| 2   | c     | 136 | ASN  |
| 2   | c     | 164 | GLN  |
| 2   | c     | 173 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | c     | 185 | ASN  |
| 3   | d     | 41  | GLN  |
| 3   | d     | 62  | GLN  |
| 3   | d     | 90  | GLN  |
| 3   | d     | 97  | ASN  |
| 3   | d     | 115 | GLN  |
| 4   | e     | 36  | ASN  |
| 4   | e     | 80  | GLN  |
| 5   | f     | 21  | GLN  |
| 5   | f     | 29  | ASN  |
| 5   | f     | 114 | HIS  |
| 5   | f     | 127 | GLN  |
| 6   | g     | 33  | GLN  |
| 6   | g     | 43  | ASN  |
| 6   | g     | 66  | ASN  |
| 7   | h     | 4   | ASN  |
| 7   | h     | 103 | ASN  |
| 8   | i     | 11  | GLN  |
| 8   | i     | 33  | ASN  |
| 8   | i     | 42  | ASN  |
| 8   | i     | 93  | ASN  |
| 8   | i     | 110 | GLN  |
| 9   | j     | 58  | ASN  |
| 9   | j     | 67  | ASN  |
| 9   | j     | 128 | ASN  |
| 9   | j     | 135 | GLN  |
| 10  | k     | 88  | ASN  |
| 10  | k     | 93  | GLN  |
| 11  | l     | 54  | GLN  |
| 13  | n     | 3   | HIS  |
| 13  | n     | 9   | GLN  |
| 13  | n     | 23  | ASN  |
| 13  | n     | 107 | ASN  |
| 14  | o     | 19  | GLN  |
| 14  | o     | 116 | GLN  |
| 15  | p     | 14  | GLN  |
| 15  | p     | 51  | ASN  |
| 15  | p     | 55  | HIS  |
| 15  | p     | 114 | ASN  |
| 16  | q     | 43  | GLN  |
| 16  | q     | 51  | GLN  |
| 17  | r     | 18  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | r     | 43  | ASN  |
| 18  | s     | 9   | HIS  |
| 18  | s     | 57  | ASN  |
| 19  | t     | 70  | HIS  |
| 20  | u     | 73  | ASN  |
| 21  | v     | 12  | GLN  |
| 21  | v     | 24  | ASN  |
| 21  | v     | 51  | GLN  |
| 21  | v     | 78  | GLN  |
| 22  | w     | 8   | ASN  |
| 22  | w     | 42  | HIS  |
| 23  | x     | 5   | GLN  |
| 23  | x     | 22  | ASN  |
| 23  | x     | 33  | HIS  |
| 24  | y     | 31  | GLN  |
| 24  | y     | 36  | GLN  |
| 24  | y     | 39  | GLN  |
| 24  | y     | 41  | HIS  |
| 24  | y     | 45  | GLN  |
| 26  | B     | 18  | HIS  |
| 28  | D     | 16  | HIS  |
| 29  | E     | 42  | HIS  |
| 30  | F     | 13  | ASN  |
| 31  | G     | 38  | HIS  |
| 31  | G     | 41  | ASN  |
| 31  | G     | 108 | GLN  |
| 31  | G     | 176 | ASN  |
| 32  | H     | 18  | ASN  |
| 32  | H     | 31  | ASN  |
| 32  | H     | 68  | HIS  |
| 32  | H     | 122 | GLN  |
| 32  | H     | 139 | ASN  |
| 33  | I     | 39  | GLN  |
| 33  | I     | 88  | ASN  |
| 33  | I     | 115 | GLN  |
| 33  | I     | 125 | ASN  |
| 34  | J     | 69  | ASN  |
| 34  | J     | 81  | GLN  |
| 36  | L     | 27  | ASN  |
| 36  | L     | 85  | GLN  |
| 36  | L     | 129 | ASN  |
| 36  | L     | 147 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | M     | 17  | GLN  |
| 38  | N     | 4   | GLN  |
| 38  | N     | 36  | GLN  |
| 38  | N     | 125 | GLN  |
| 39  | O     | 64  | GLN  |
| 40  | P     | 27  | ASN  |
| 40  | P     | 39  | ASN  |
| 40  | P     | 118 | ASN  |
| 41  | Q     | 45  | ASN  |
| 42  | R     | 7   | ASN  |
| 42  | R     | 51  | GLN  |
| 43  | S     | 61  | ASN  |
| 43  | S     | 65  | GLN  |
| 44  | T     | 36  | ASN  |
| 44  | T     | 79  | GLN  |
| 45  | U     | 9   | HIS  |
| 45  | U     | 79  | ASN  |
| 46  | V     | 8   | GLN  |
| 46  | V     | 44  | HIS  |
| 47  | W     | 30  | ASN  |
| 47  | W     | 53  | GLN  |
| 48  | X     | 56  | HIS  |
| 49  | Y     | 20  | ASN  |
| 49  | Y     | 51  | ASN  |
| 49  | Y     | 69  | ASN  |
| 49  | Y     | 77  | ASN  |
| 49  | Y     | 83  | ASN  |
| 51  | a     | 24  | ASN  |
| 51  | a     | 67  | HIS  |
| 51  | a     | 160 | GLN  |
| 51  | a     | 168 | ASN  |
| 51  | a     | 188 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 52  | 3     | 1538/1539 (99%) | 138 (8%)          | 2 (0%)          |
| 53  | 1     | 2902/2903 (99%) | 335 (11%)         | 11 (0%)         |
| 54  | 2     | 119/120 (99%)   | 10 (8%)           | 1 (0%)          |
| 55  | 5     | 76/77 (98%)     | 8 (10%)           | 0               |
| 55  | 6     | 76/77 (98%)     | 8 (10%)           | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 56  | 4     | 17/18 (94%)     | 3 (17%)           | 0               |
| 57  | 7     | 75/76 (98%)     | 11 (14%)          | 0               |
| All | All   | 4803/4810 (99%) | 513 (10%)         | 14 (0%)         |

All (513) 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     | 95  | C    |
| 52  | 3     | 100 | G    |
| 52  | 3     | 130 | A    |
| 52  | 3     | 144 | G    |
| 52  | 3     | 183 | C    |
| 52  | 3     | 184 | G    |
| 52  | 3     | 197 | A    |
| 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     | 355 | C    |
| 52  | 3     | 367 | U    |
| 52  | 3     | 372 | C    |
| 52  | 3     | 411 | A    |
| 52  | 3     | 412 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | 3     | 413 | G    |
| 52  | 3     | 429 | U    |
| 52  | 3     | 467 | U    |
| 52  | 3     | 479 | U    |
| 52  | 3     | 484 | G    |
| 52  | 3     | 485 | U    |
| 52  | 3     | 486 | U    |
| 52  | 3     | 497 | G    |
| 52  | 3     | 518 | C    |
| 52  | 3     | 532 | A    |
| 52  | 3     | 547 | A    |
| 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     | 666 | G    |
| 52  | 3     | 688 | G    |
| 52  | 3     | 703 | G    |
| 52  | 3     | 723 | U    |
| 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     | 829 | 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     | 926 | G    |
| 52  | 3     | 934 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 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    |
| 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     | 1225 | A    |
| 52  | 3     | 1238 | A    |
| 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    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 52  | 3     | 1300 | G    |
| 52  | 3     | 1317 | C    |
| 52  | 3     | 1346 | A    |
| 52  | 3     | 1347 | G    |
| 52  | 3     | 1363 | A    |
| 52  | 3     | 1378 | C    |
| 52  | 3     | 1381 | U    |
| 52  | 3     | 1395 | C    |
| 52  | 3     | 1446 | A    |
| 52  | 3     | 1448 | C    |
| 52  | 3     | 1452 | C    |
| 52  | 3     | 1492 | A    |
| 52  | 3     | 1503 | A    |
| 52  | 3     | 1506 | U    |
| 52  | 3     | 1517 | G    |
| 52  | 3     | 1529 | G    |
| 52  | 3     | 1530 | G    |
| 52  | 3     | 1534 | A    |
| 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     | 98   | G    |
| 53  | 1     | 102  | U    |
| 53  | 1     | 119  | A    |
| 53  | 1     | 120  | U    |
| 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    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 1     | 181 | A    |
| 53  | 1     | 196 | A    |
| 53  | 1     | 216 | A    |
| 53  | 1     | 219 | A    |
| 53  | 1     | 221 | A    |
| 53  | 1     | 222 | A    |
| 53  | 1     | 224 | U    |
| 53  | 1     | 228 | C    |
| 53  | 1     | 229 | C    |
| 53  | 1     | 248 | G    |
| 53  | 1     | 249 | C    |
| 53  | 1     | 255 | A    |
| 53  | 1     | 265 | A    |
| 53  | 1     | 266 | G    |
| 53  | 1     | 276 | U    |
| 53  | 1     | 278 | A    |
| 53  | 1     | 281 | C    |
| 53  | 1     | 294 | A    |
| 53  | 1     | 301 | G    |
| 53  | 1     | 311 | A    |
| 53  | 1     | 312 | G    |
| 53  | 1     | 323 | C    |
| 53  | 1     | 329 | G    |
| 53  | 1     | 330 | A    |
| 53  | 1     | 361 | G    |
| 53  | 1     | 367 | G    |
| 53  | 1     | 371 | A    |
| 53  | 1     | 372 | G    |
| 53  | 1     | 373 | U    |
| 53  | 1     | 386 | G    |
| 53  | 1     | 387 | U    |
| 53  | 1     | 404 | A    |
| 53  | 1     | 406 | G    |
| 53  | 1     | 411 | G    |
| 53  | 1     | 422 | A    |
| 53  | 1     | 424 | G    |
| 53  | 1     | 451 | U    |
| 53  | 1     | 455 | C    |
| 53  | 1     | 457 | A    |
| 53  | 1     | 458 | G    |
| 53  | 1     | 481 | G    |
| 53  | 1     | 491 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 1     | 492 | A    |
| 53  | 1     | 504 | A    |
| 53  | 1     | 505 | A    |
| 53  | 1     | 529 | A    |
| 53  | 1     | 531 | C    |
| 53  | 1     | 532 | A    |
| 53  | 1     | 543 | G    |
| 53  | 1     | 545 | U    |
| 53  | 1     | 563 | A    |
| 53  | 1     | 573 | U    |
| 53  | 1     | 588 | U    |
| 53  | 1     | 603 | A    |
| 53  | 1     | 616 | A    |
| 53  | 1     | 627 | A    |
| 53  | 1     | 637 | A    |
| 53  | 1     | 645 | C    |
| 53  | 1     | 646 | U    |
| 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     | 859 | G    |
| 53  | 1     | 860 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 878  | A    |
| 53  | 1     | 885  | C    |
| 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     | 959  | A    |
| 53  | 1     | 961  | C    |
| 53  | 1     | 974  | G    |
| 53  | 1     | 983  | A    |
| 53  | 1     | 995  | C    |
| 53  | 1     | 996  | A    |
| 53  | 1     | 1012 | U    |
| 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     | 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    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 1157 | G    |
| 53  | 1     | 1175 | A    |
| 53  | 1     | 1177 | G    |
| 53  | 1     | 1180 | U    |
| 53  | 1     | 1212 | G    |
| 53  | 1     | 1250 | 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     | 1301 | A    |
| 53  | 1     | 1302 | A    |
| 53  | 1     | 1329 | U    |
| 53  | 1     | 1330 | C    |
| 53  | 1     | 1332 | G    |
| 53  | 1     | 1345 | C    |
| 53  | 1     | 1365 | A    |
| 53  | 1     | 1378 | A    |
| 53  | 1     | 1379 | U    |
| 53  | 1     | 1383 | A    |
| 53  | 1     | 1395 | 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     | 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     | 1560 | G    |
| 53  | 1     | 1569 | A    |
| 53  | 1     | 1581 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 1584 | U    |
| 53  | 1     | 1608 | A    |
| 53  | 1     | 1611 | C    |
| 53  | 1     | 1616 | A    |
| 53  | 1     | 1647 | U    |
| 53  | 1     | 1648 | U    |
| 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    |
| 53  | 1     | 1764 | C    |
| 53  | 1     | 1773 | A    |
| 53  | 1     | 1780 | A    |
| 53  | 1     | 1791 | A    |
| 53  | 1     | 1800 | C    |
| 53  | 1     | 1801 | A    |
| 53  | 1     | 1808 | A    |
| 53  | 1     | 1816 | C    |
| 53  | 1     | 1829 | A    |
| 53  | 1     | 1871 | A    |
| 53  | 1     | 1901 | A    |
| 53  | 1     | 1906 | G    |
| 53  | 1     | 1907 | G    |
| 53  | 1     | 1913 | A    |
| 53  | 1     | 1914 | C    |
| 53  | 1     | 1929 | G    |
| 53  | 1     | 1930 | G    |
| 53  | 1     | 1937 | A    |
| 53  | 1     | 1938 | A    |
| 53  | 1     | 1944 | U    |
| 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    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 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     | 2096 | C    |
| 53  | 1     | 2110 | G    |
| 53  | 1     | 2111 | U    |
| 53  | 1     | 2112 | G    |
| 53  | 1     | 2118 | U    |
| 53  | 1     | 2119 | A    |
| 53  | 1     | 2132 | U    |
| 53  | 1     | 2133 | G    |
| 53  | 1     | 2145 | C    |
| 53  | 1     | 2162 | G    |
| 53  | 1     | 2172 | U    |
| 53  | 1     | 2173 | A    |
| 53  | 1     | 2189 | U    |
| 53  | 1     | 2198 | A    |
| 53  | 1     | 2203 | U    |
| 53  | 1     | 2204 | G    |
| 53  | 1     | 2212 | A    |
| 53  | 1     | 2213 | U    |
| 53  | 1     | 2225 | A    |
| 53  | 1     | 2259 | U    |
| 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    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 2383 | G    |
| 53  | 1     | 2385 | C    |
| 53  | 1     | 2392 | A    |
| 53  | 1     | 2402 | U    |
| 53  | 1     | 2406 | A    |
| 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    |
| 53  | 1     | 2502 | G    |
| 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     | 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     | 2764 | A    |
| 53  | 1     | 2765 | A    |
| 53  | 1     | 2778 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 2779 | U    |
| 53  | 1     | 2791 | G    |
| 53  | 1     | 2794 | C    |
| 53  | 1     | 2797 | U    |
| 53  | 1     | 2799 | A    |
| 53  | 1     | 2800 | A    |
| 53  | 1     | 2809 | A    |
| 53  | 1     | 2820 | A    |
| 53  | 1     | 2821 | A    |
| 53  | 1     | 2833 | U    |
| 53  | 1     | 2849 | U    |
| 53  | 1     | 2850 | A    |
| 53  | 1     | 2867 | G    |
| 53  | 1     | 2868 | A    |
| 53  | 1     | 2872 | A    |
| 53  | 1     | 2880 | C    |
| 53  | 1     | 2883 | A    |
| 53  | 1     | 2884 | U    |
| 54  | 2     | 4    | 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     | 9    | G    |
| 55  | 5     | 18   | G    |
| 55  | 5     | 19   | G    |
| 55  | 5     | 20   | U    |
| 55  | 5     | 47   | U    |
| 55  | 5     | 48   | C    |
| 55  | 5     | 61   | C    |
| 55  | 5     | 76   | A    |
| 55  | 6     | 6    | G    |
| 55  | 6     | 9    | G    |
| 55  | 6     | 18   | G    |
| 55  | 6     | 19   | G    |
| 55  | 6     | 20   | U    |
| 55  | 6     | 47   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | 6     | 48  | C    |
| 55  | 6     | 61  | C    |
| 56  | 4     | 12  | A    |
| 56  | 4     | 13  | A    |
| 56  | 4     | 19  | C    |
| 57  | 7     | 17  | C    |
| 57  | 7     | 19  | G    |
| 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    |
| 57  | 7     | 74  | C    |

All (14) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 52  | 3     | 1190 | G    |
| 52  | 3     | 1201 | A    |
| 53  | 1     | 227  | A    |
| 53  | 1     | 372  | G    |
| 53  | 1     | 421  | C    |
| 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 ⓘ

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

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 59  | PHE  | 7     | 101 | 57   | 10,11,12     | 0.69 | 0           | 8,13,15     | 0.29 | 0           |
| 58  | FME  | 5     | 101 | 55   | 8,9,10       | 0.50 | 0           | 8,9,11      | 0.82 | 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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 59  | PHE  | 7     | 101 | 57   | -       | 0/5/6/8  | 0/1/1/1 |
| 58  | FME  | 5     | 101 | 55   | -       | 2/7/9/11 | -       |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21639. 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

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit

This section was not generated.