



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:48 AM UTC

PDB ID : 6WD2 / pdb\_00006wd2  
EMDB ID : EMD-21621  
Title : Cryo-EM of elongating ribosome with EF-Tu\*GTP elucidates tRNA proof-reading (Cognate Structure II-A)  
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  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

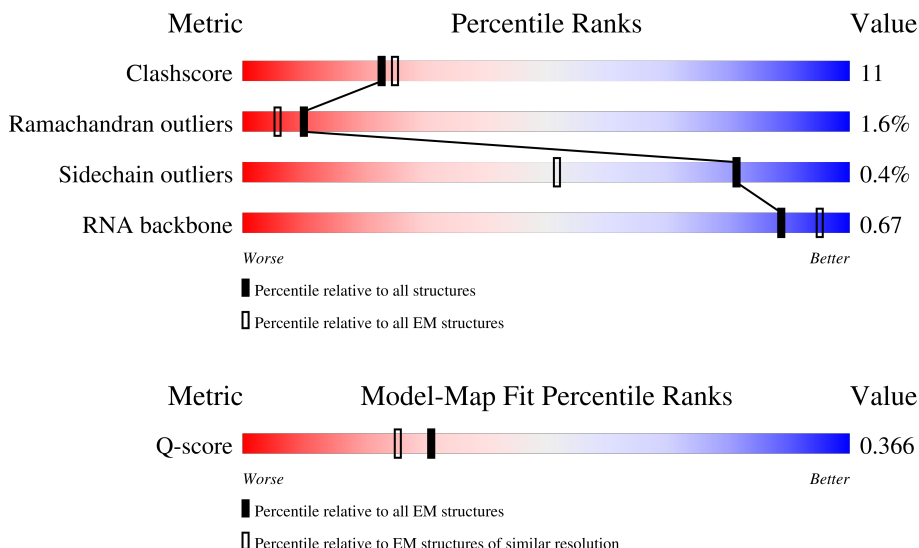
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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.



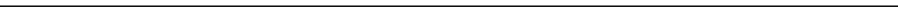
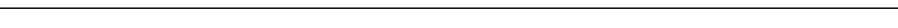
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 12797 ( 3.10 - 4.10 )                                    |

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

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

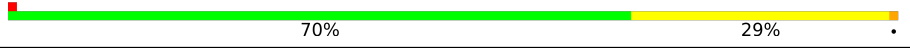
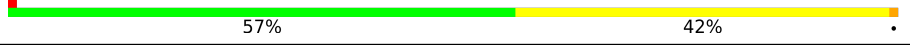
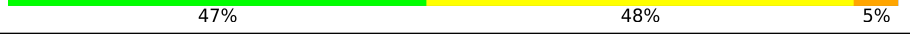
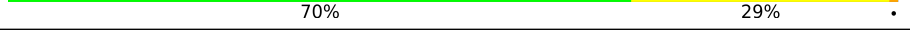
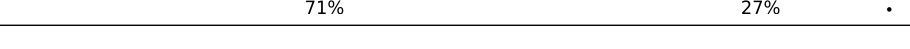
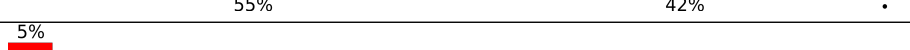
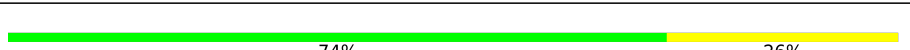
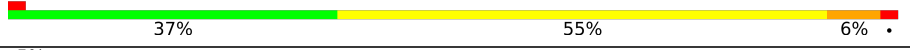
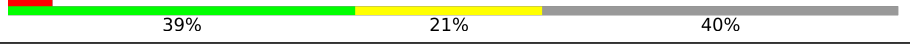
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| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 4   | e     | 177    |  70% 29% .        |
| 5   | f     | 176    |  80% 20% .        |
| 6   | g     | 149    |  8% 63% 35% .     |
| 7   | h     | 131    |  13% 50% 43% 5% . |
| 8   | i     | 141    |  11% 65% 34% ..   |
| 9   | j     | 142    |  78% 21% .        |
| 10  | k     | 122    |  64% 32% .        |
| 11  | l     | 143    |  72% 27% .        |
| 12  | m     | 136    |  69% 29% .        |
| 13  | n     | 120    |  69% 31% .        |
| 14  | o     | 116    |  71% 28% .        |
| 15  | p     | 114    |  67% 32% .        |
| 16  | q     | 117    |  75% 22% .      |
| 17  | r     | 103    |  67% 29% .      |
| 18  | s     | 110    |  72% 26% .      |
| 19  | t     | 93     |  68% 31% .      |
| 20  | u     | 102    |  74% 25% .      |
| 21  | v     | 94     |  66% 34% .      |
| 22  | w     | 75     |  80% 20% .      |
| 23  | x     | 77     |  70% 30% .      |
| 24  | y     | 63     |  56% 43% .      |
| 25  | z     | 58     |  74% 26% .      |
| 26  | B     | 56     |  75% 23% .      |
| 27  | C     | 50     |  54% 44% .      |
| 28  | D     | 46     |  72% 28% .      |

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

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| Mol | Chain | Length | Quality of chain                                                              |
|-----|-------|--------|-------------------------------------------------------------------------------|
| 54  | 2     | 120    | <div><div></div><div>56%</div><div>38%</div><div>7%</div></div>               |
| 55  | 5     | 77     | <div><div></div><div>73%</div><div>25%</div><div></div></div>                 |
| 55  | 6     | 77     | <div><div></div><div>53%</div><div>43%</div><div></div></div>                 |
| 56  | 4     | 18     | <div><div></div><div>11%</div><div>67%</div><div>28%</div><div>6%</div></div> |
| 57  | 7     | 76     | <div><div></div><div>53%</div><div>37%</div><div>11%</div></div>              |
| 58  | 8     | 400    | <div><div></div><div>63%</div><div>33%</div><div></div></div>                 |

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 153282 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

- 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 1370526515 |

- 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 | 76 | 120 | 17 |         |       |

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

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

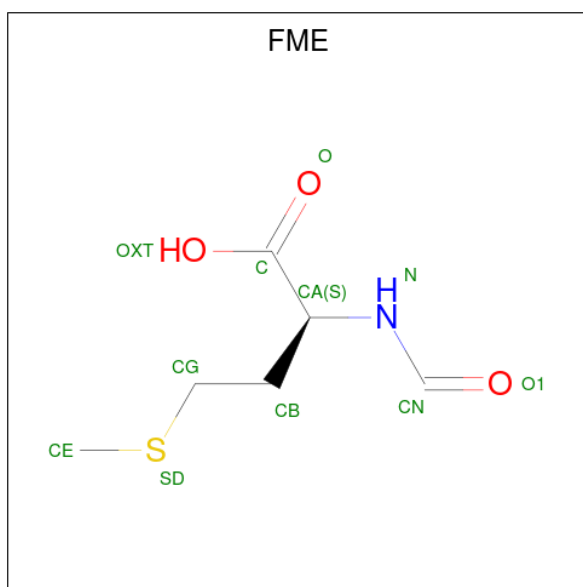
- Molecule 58 is a protein called Elongation factor Tu.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 58  | 8     | 392      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3028  | 1915 | 521 | 579 | 13 |         |       |

There are 7 discrepancies between the modelled and reference sequences:

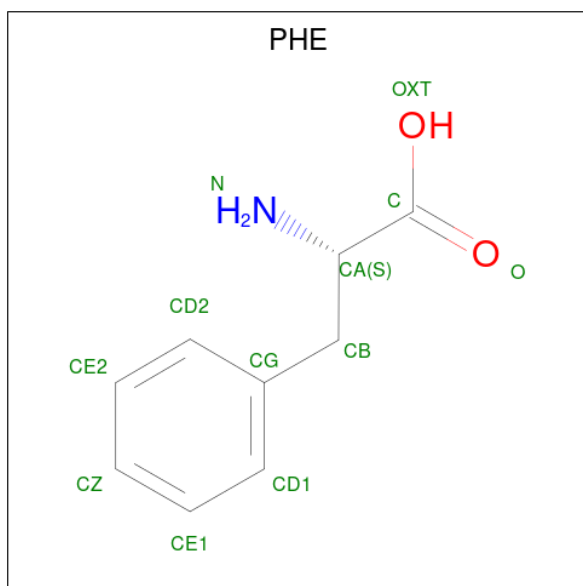
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| 8     | 395     | SER      | -      | expression tag | UNP E2QFJ4 |
| 8     | 396     | HIS      | -      | expression tag | UNP E2QFJ4 |
| 8     | 397     | HIS      | -      | expression tag | UNP E2QFJ4 |
| 8     | 398     | HIS      | -      | expression tag | UNP E2QFJ4 |
| 8     | 399     | HIS      | -      | expression tag | UNP E2QFJ4 |
| 8     | 400     | HIS      | -      | expression tag | UNP E2QFJ4 |
| 8     | 401     | HIS      | -      | expression tag | UNP E2QFJ4 |

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



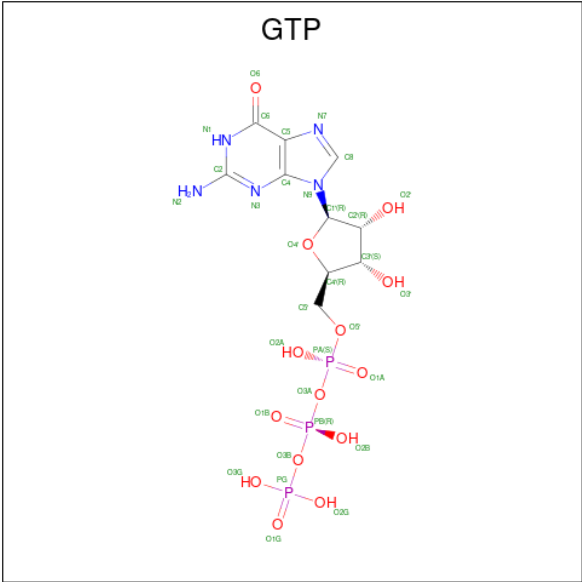
| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 59  | 5     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 10    | 6 | 1 | 2 | 1 |         |

- Molecule 60 is PHENYLALANINE (CCD ID: PHE) (formula:  $C_9H_{11}NO_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 60  | 7     | 1        | Total | C | N | O | 0       |
|     |       |          | 11    | 9 | 1 | 1 |         |

- Molecule 61 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



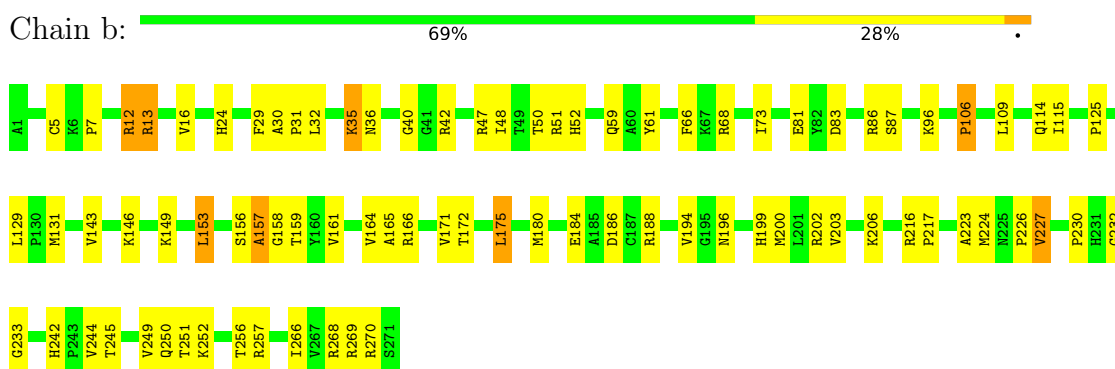
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 61  | 8     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |



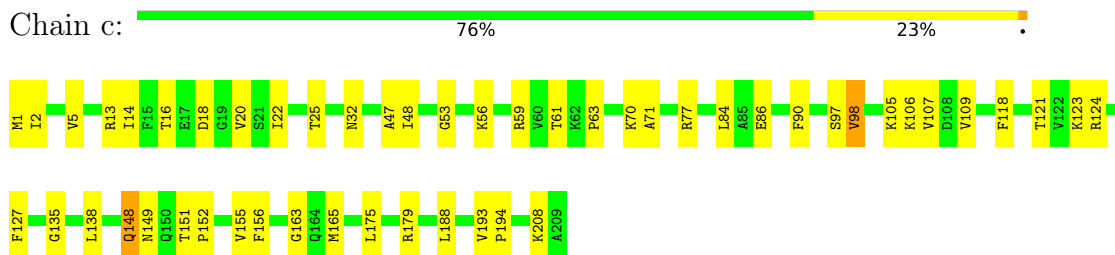
### 3 Residue-property plots

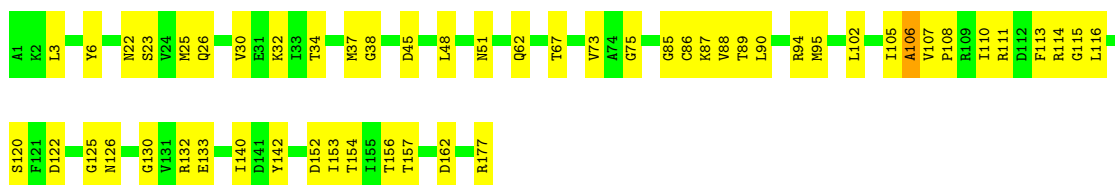
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 50S ribosomal protein L2



- Molecule 2: 50S ribosomal protein L3





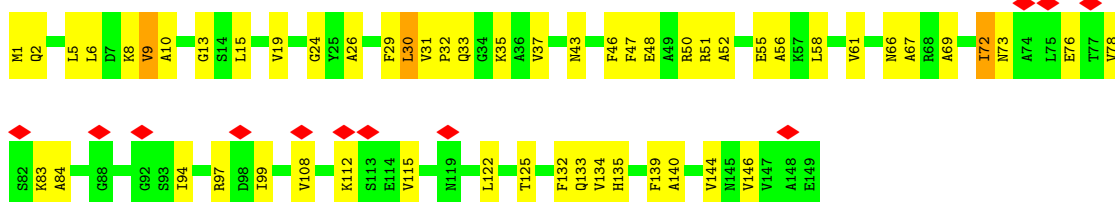
• Molecule 5: 50S ribosomal protein L6

Chain f: 80% 20% .



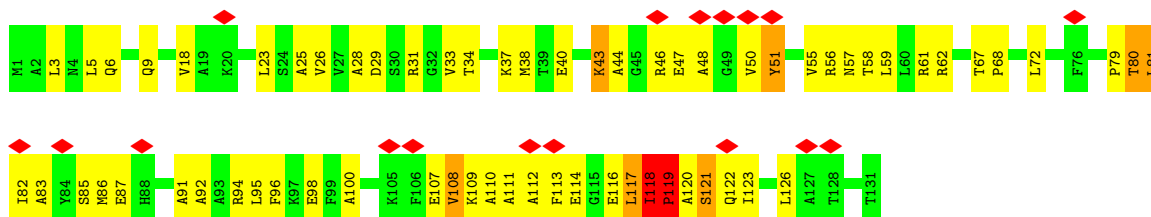
• Molecule 6: 50S ribosomal protein L9

Chain g: 8% 63% 35% .



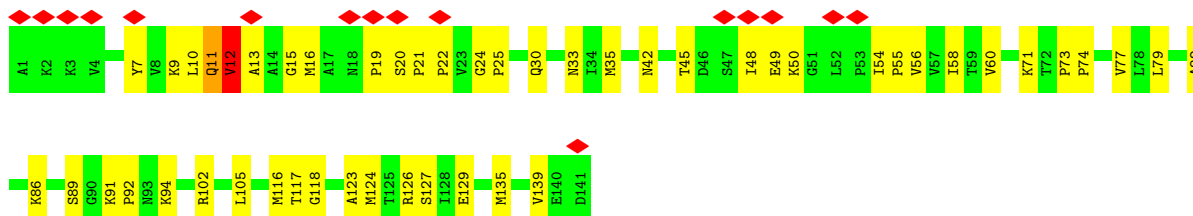
• Molecule 7: 50S ribosomal protein L10

Chain h: 13% 50% 43% 5% .



• Molecule 8: 50S ribosomal protein L11

Chain i: 11% 65% 34% .



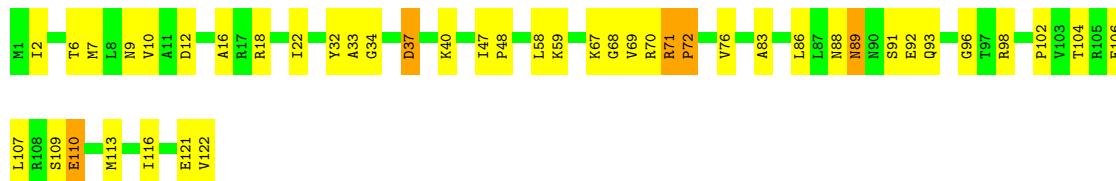
- Molecule 9: 50S ribosomal protein L13

Chain j:  78% 21%



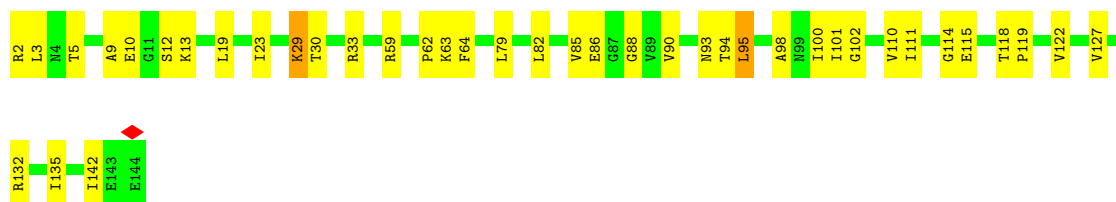
- Molecule 10: 50S ribosomal protein L14

Chain k:  64% 32%



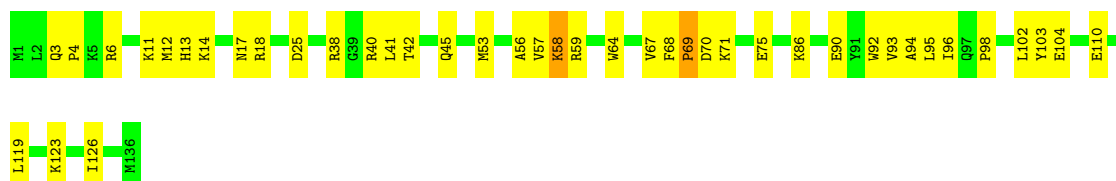
- Molecule 11: 50S ribosomal protein L15

Chain l:  72% 27%



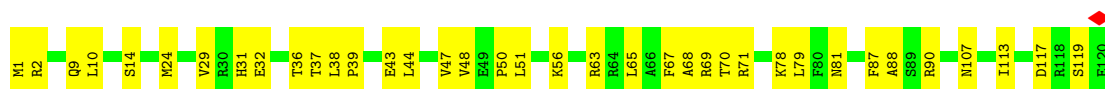
- Molecule 12: 50S ribosomal protein L16

Chain m:  69% 29%



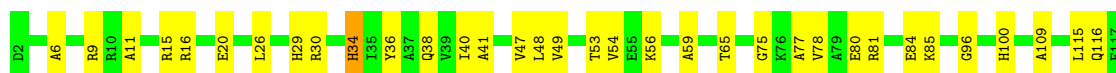
- Molecule 13: 50S ribosomal protein L17

Chain n:  69% 31%

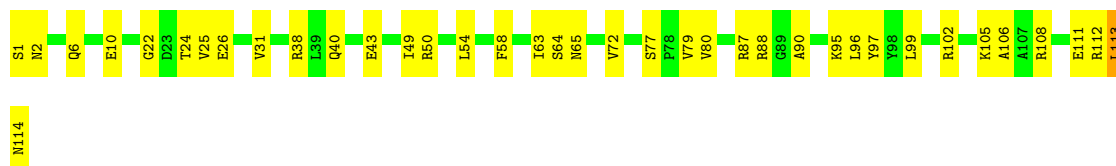


- Molecule 14: 50S ribosomal protein L18

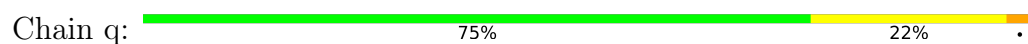
Chain o:  71% 28%



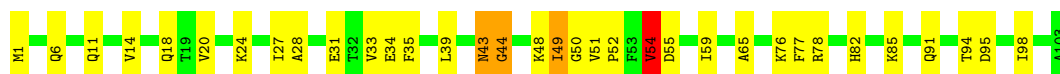
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23

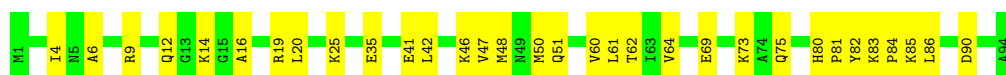


- Molecule 20: 50S ribosomal protein L24



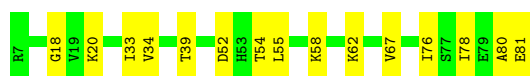
- Molecule 21: 50S ribosomal protein L25

Chain v:  66% 34%



- Molecule 22: 50S ribosomal protein L27

Chain w:  80% 20%



- Molecule 23: 50S ribosomal protein L28

Chain x:  70% 30%



- Molecule 24: 50S ribosomal protein L29

Chain y:  56% 43% .



- Molecule 25: 50S ribosomal protein L30

Chain z:  74% 26%



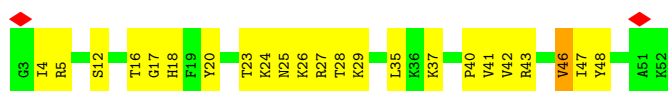
- Molecule 26: 50S ribosomal protein L32

Chain B:  75% 23% .



- Molecule 27: 50S ribosomal protein L33

Chain C:  54% 44% .



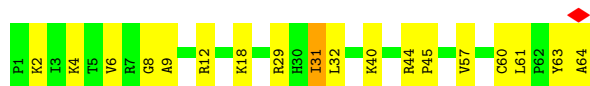
- Molecule 28: 50S ribosomal protein L34

Chain D:  72% 28%



- Molecule 29: 50S ribosomal protein L35

Chain E:  72% 27%



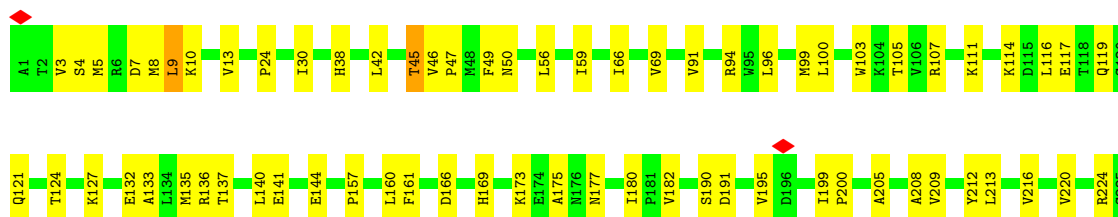
- Molecule 30: 50S ribosomal protein L36

Chain F:  53% 45%



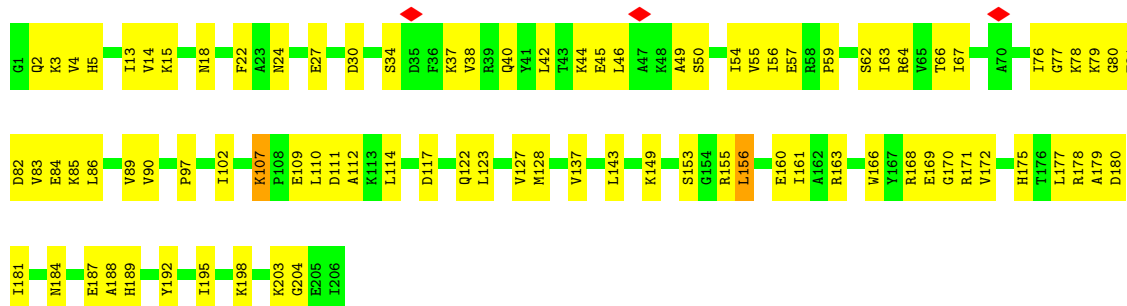
- Molecule 31: 30S ribosomal protein S2

Chain G:  70% 29%



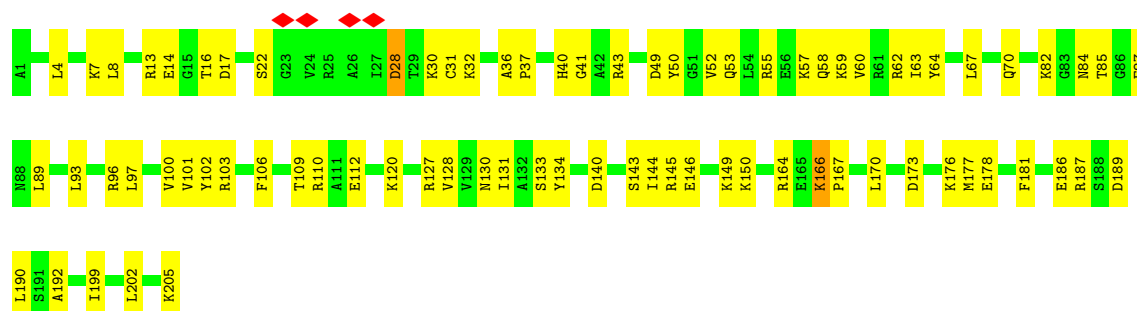
- Molecule 32: 30S ribosomal protein S3

Chain H:  57% 42%



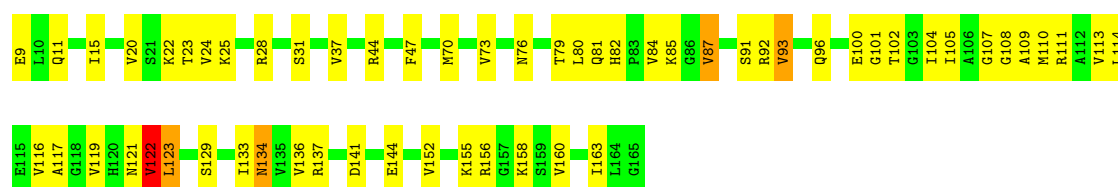
- Molecule 33: 30S ribosomal protein S4

Chain I:  62% 37%



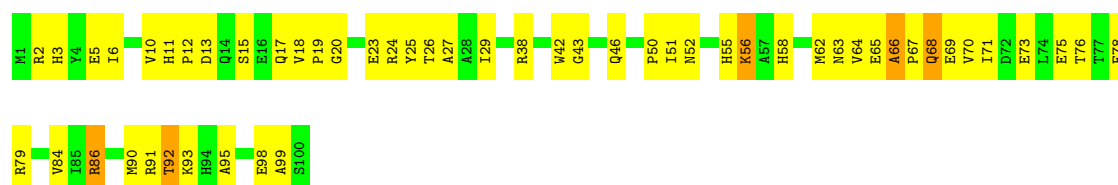
- Molecule 34: 30S ribosomal protein S5

Chain J: 63% 34%



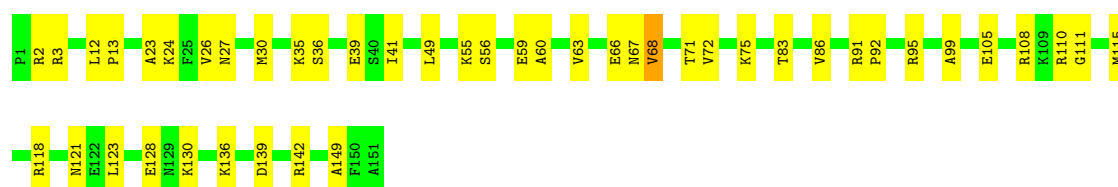
- Molecule 35: 30S ribosomal protein S6

Chain K: 47% 48% 5%



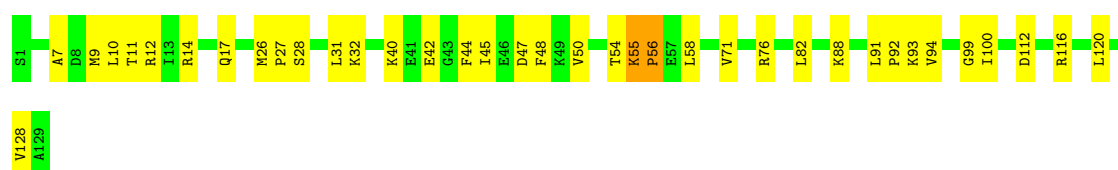
- Molecule 36: 30S ribosomal protein S7

Chain L: 70% 29%

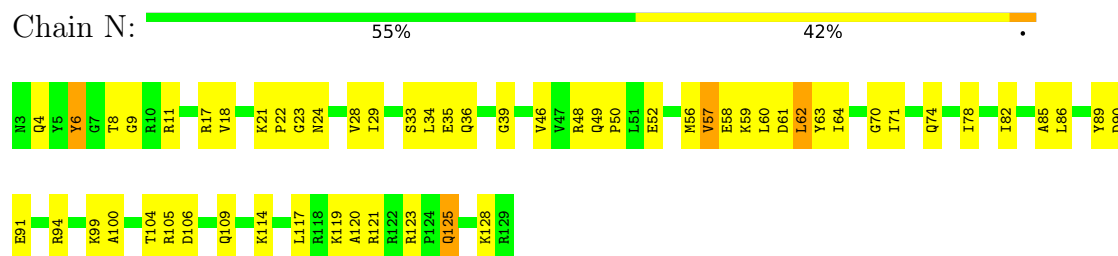


- Molecule 37: 30S ribosomal protein S8

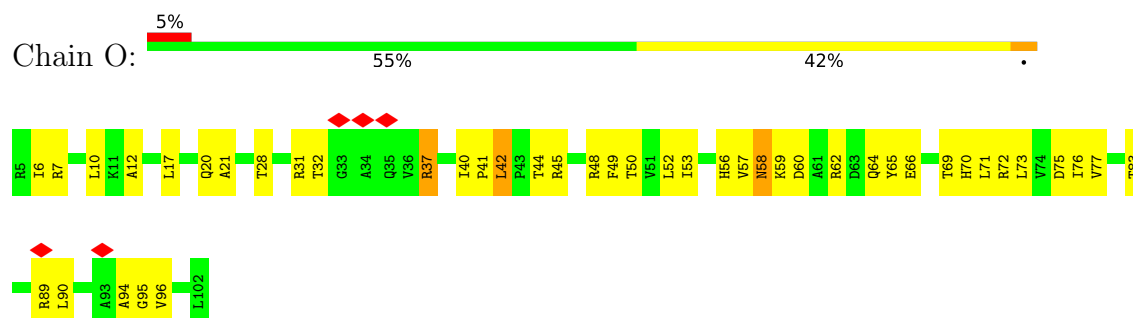
Chain M: 71% 27%



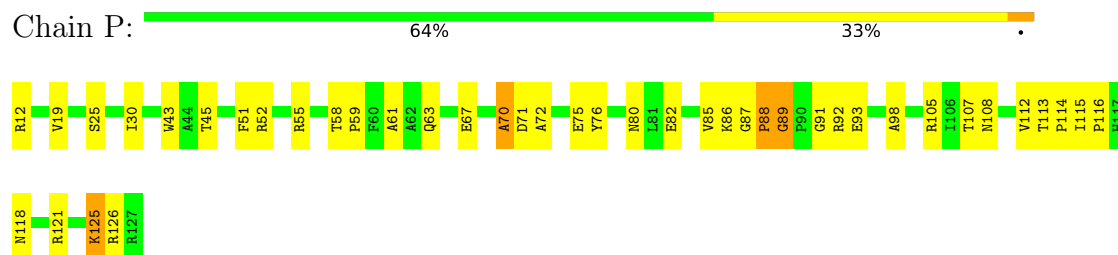
- Molecule 38: 30S ribosomal protein S9



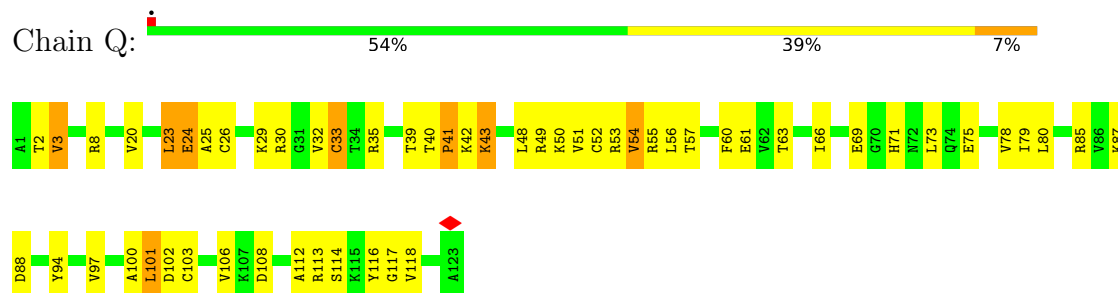
- Molecule 39: 30S ribosomal protein S10



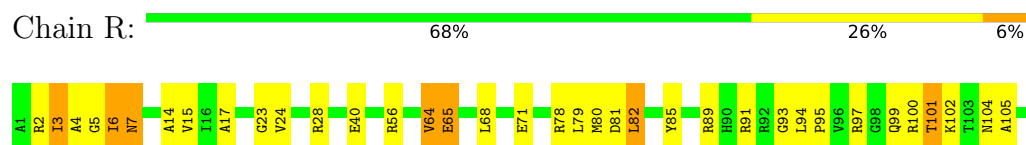
- Molecule 40: 30S ribosomal protein S11



- Molecule 41: 30S ribosomal protein S12



- Molecule 42: 30S ribosomal protein S13



- Molecule 43: 30S ribosomal protein S14



Chain S:  60% 40%



- Molecule 44: 30S ribosomal protein S15

Chain T:  74% 26%



- Molecule 45: 30S ribosomal protein S16

Chain U:  60% 37% .



- Molecule 46: 30S ribosomal protein S17

Chain V:  56% 42% .



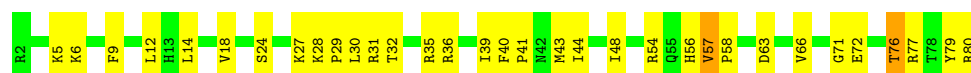
- Molecule 47: 30S ribosomal protein S18

Chain W:  69% 29% .



- Molecule 48: 30S ribosomal protein S19

Chain X:  58% 39% .

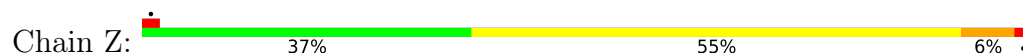


- Molecule 49: 30S ribosomal protein S20

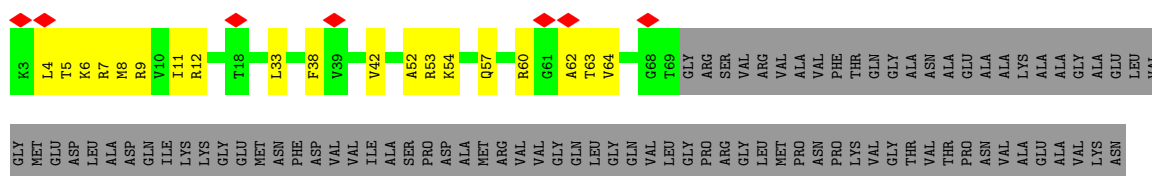
Chain Y:  67% 33%



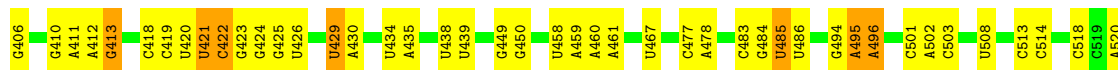
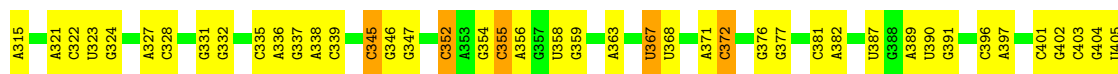
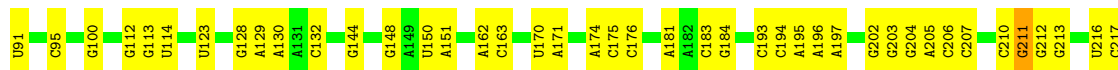
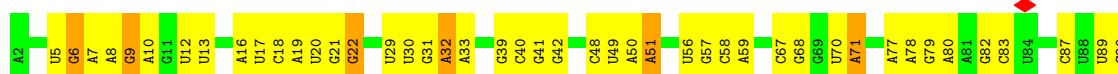
- Molecule 50: 30S ribosomal protein S21

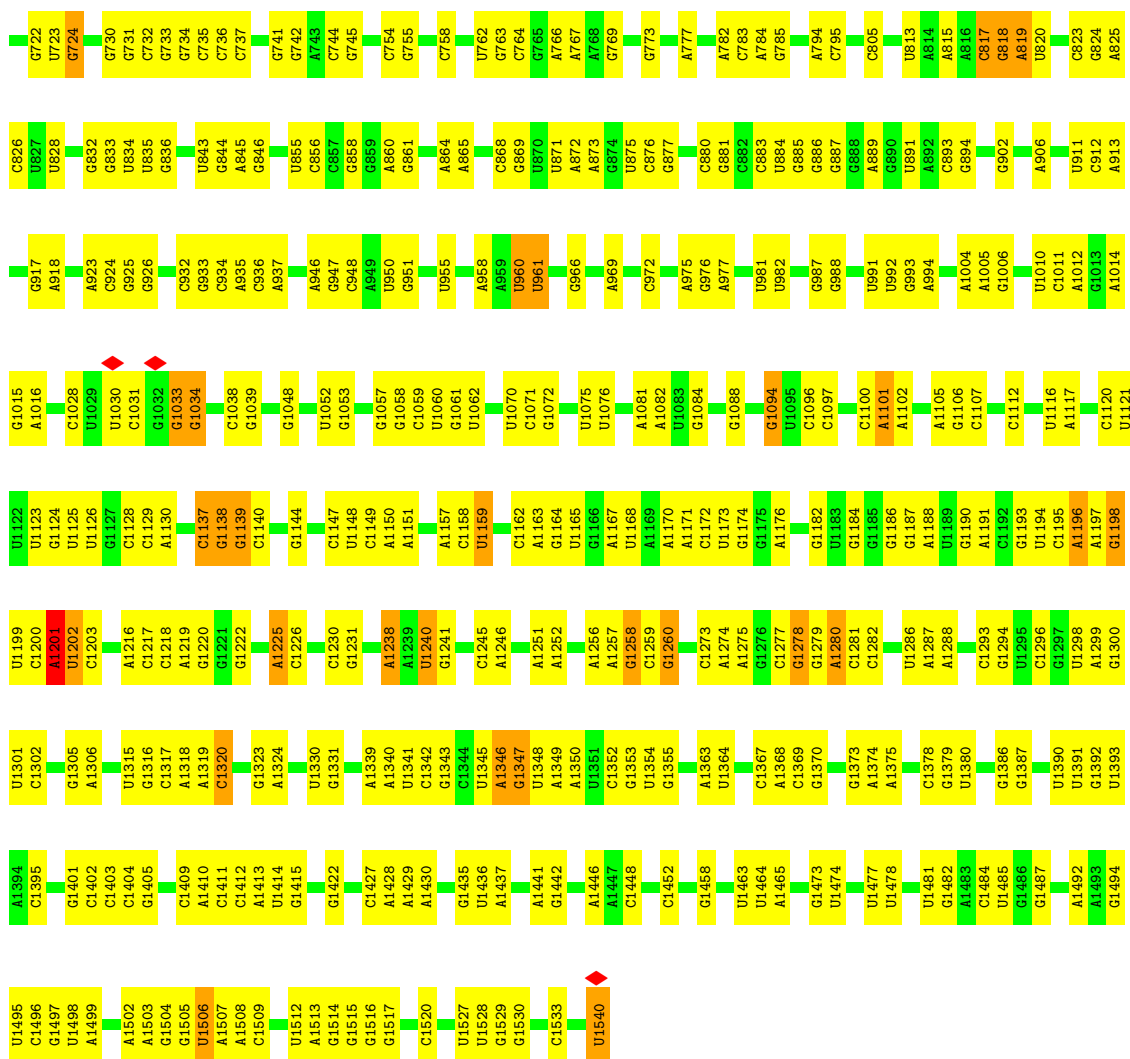


- Molecule 51: 50S ribosomal protein L1



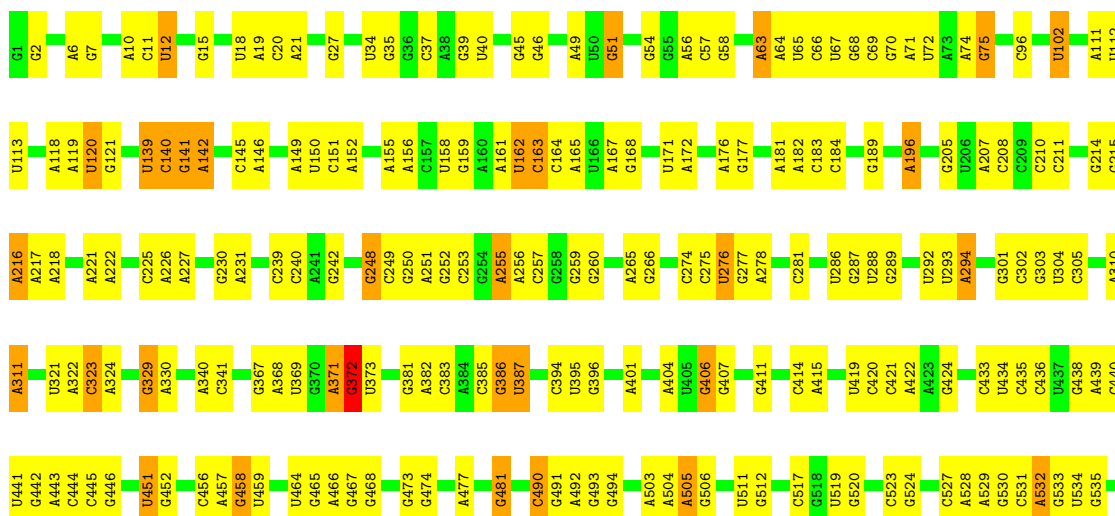
- Molecule 52: 16S ribosomal RNA



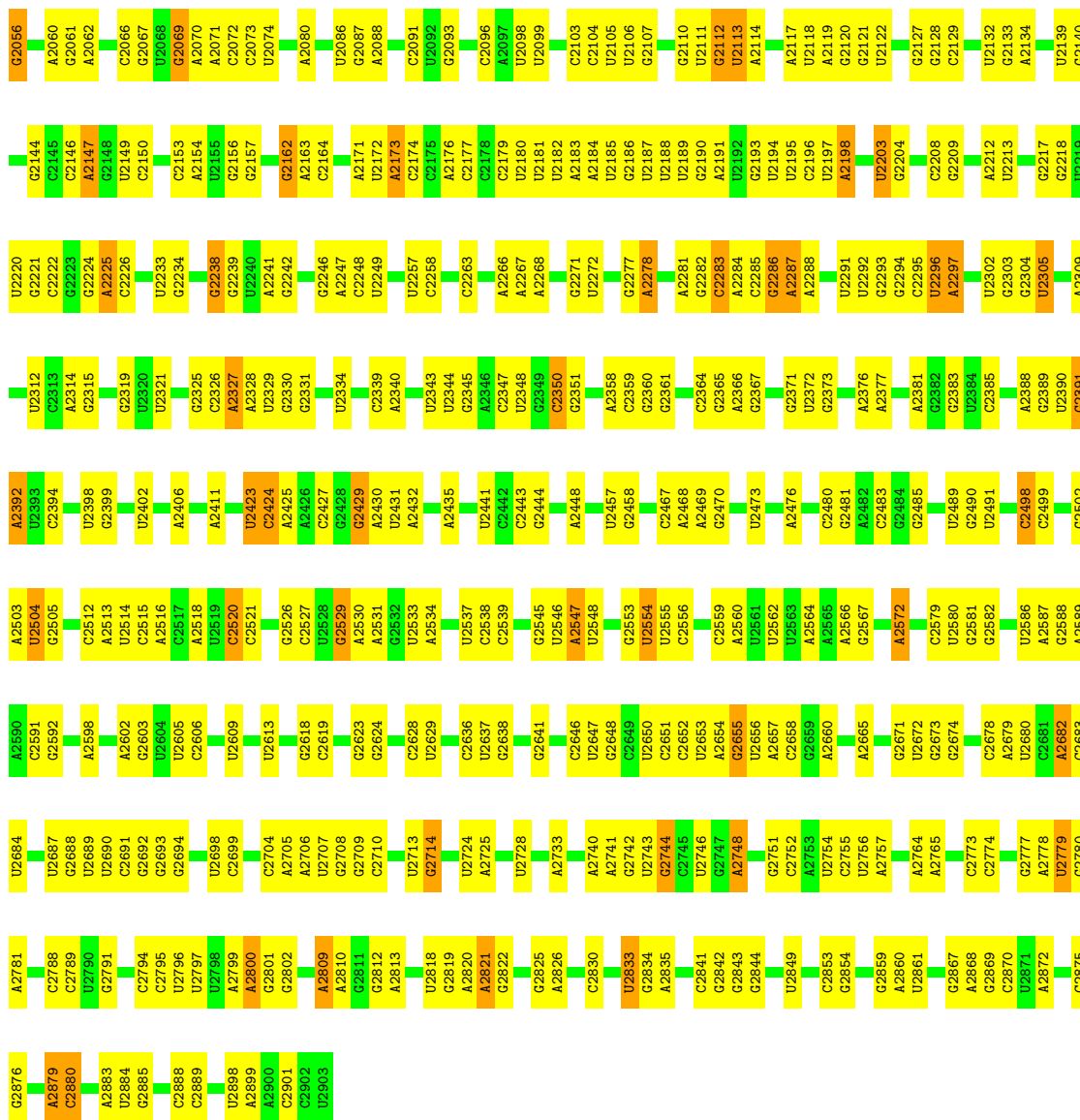


• Molecule 53: 23S ribosomal RNA

Chain 1: 56% 38% 5%

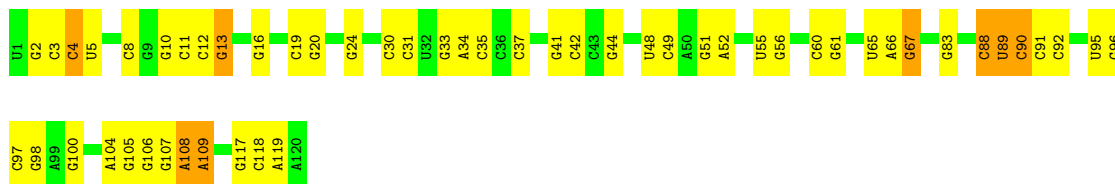






• Molecule 54: 5S ribosomal RNA

Chain 2: 56% 38% 7%



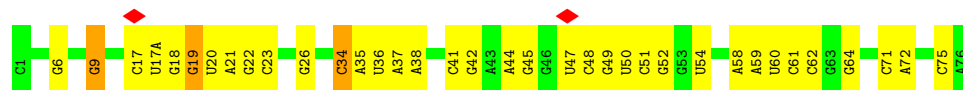
• Molecule 55: tRNA<sup>fMet</sup>

Chain 5: 73% 25%



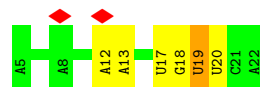
- Molecule 55: tRNA<sup>fMet</sup>

Chain 6: 



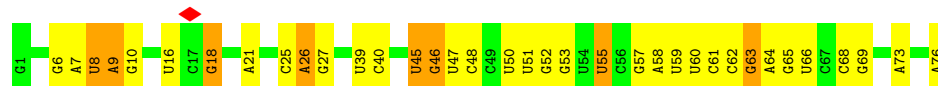
- Molecule 56: mRNA

Chain 4: 



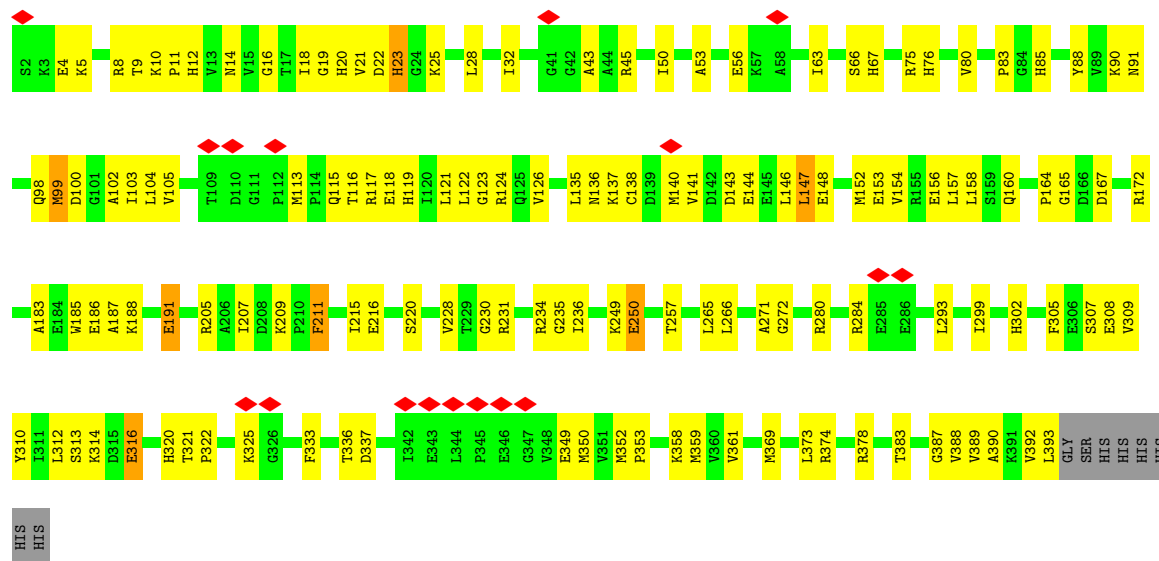
- Molecule 57: tRNA<sup>Phe</sup>

Chain 7: 



- Molecule 58: Elongation factor Tu

Chain 8: 



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 7320                                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 35                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 19.159                                  | Depositor |
| Minimum map value                    | -11.373                                 | Depositor |
| Average map value                    | 0.114                                   | Depositor |
| Map value standard deviation         | 0.888                                   | Depositor |
| Recommended contour level            | 1                                       | Depositor |
| Map size (Å)                         | 383.904, 383.904, 383.904               | wwPDB     |
| Map dimensions                       | 288, 288, 288                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.333, 1.333, 1.333                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 1   | b     | 0.30         | 0/2122  | 0.94        | 9/2852 (0.3%) |
| 2   | c     | 0.29         | 0/1586  | 0.84        | 2/2134 (0.1%) |
| 3   | d     | 0.28         | 0/1571  | 0.87        | 3/2113 (0.1%) |
| 4   | e     | 0.29         | 0/1435  | 0.86        | 3/1926 (0.2%) |
| 5   | f     | 0.29         | 0/1343  | 0.81        | 0/1816        |
| 6   | g     | 0.32         | 0/1122  | 0.99        | 5/1515 (0.3%) |
| 7   | h     | 0.34         | 0/1002  | 1.04        | 7/1350 (0.5%) |
| 8   | i     | 0.36         | 0/1046  | 0.94        | 2/1410 (0.1%) |
| 9   | j     | 0.30         | 0/1152  | 0.86        | 2/1551 (0.1%) |
| 10  | k     | 0.29         | 0/948   | 1.01        | 6/1268 (0.5%) |
| 11  | l     | 0.30         | 0/1054  | 0.99        | 4/1403 (0.3%) |
| 12  | m     | 0.30         | 0/1093  | 0.88        | 2/1460 (0.1%) |
| 13  | n     | 0.30         | 0/974   | 0.99        | 7/1301 (0.5%) |
| 14  | o     | 0.28         | 0/902   | 0.83        | 1/1209 (0.1%) |
| 15  | p     | 0.30         | 0/929   | 0.85        | 1/1242 (0.1%) |
| 16  | q     | 0.28         | 0/960   | 0.90        | 3/1278 (0.2%) |
| 17  | r     | 0.28         | 0/829   | 0.86        | 4/1107 (0.4%) |
| 18  | s     | 0.28         | 0/864   | 0.89        | 3/1156 (0.3%) |
| 19  | t     | 0.29         | 0/745   | 0.79        | 0/994         |
| 20  | u     | 0.30         | 0/788   | 0.88        | 3/1051 (0.3%) |
| 21  | v     | 0.28         | 0/766   | 0.87        | 0/1025        |
| 22  | w     | 0.27         | 0/582   | 0.83        | 1/769 (0.1%)  |
| 23  | x     | 0.29         | 0/635   | 0.83        | 0/848         |
| 24  | y     | 0.27         | 0/510   | 0.85        | 1/677 (0.1%)  |
| 25  | z     | 0.29         | 0/453   | 0.81        | 0/605         |
| 26  | B     | 0.28         | 0/450   | 0.78        | 1/599 (0.2%)  |
| 27  | C     | 0.31         | 0/417   | 0.80        | 1/554 (0.2%)  |
| 28  | D     | 0.32         | 0/380   | 0.84        | 0/498         |
| 29  | E     | 0.29         | 0/513   | 0.82        | 0/676         |
| 30  | F     | 0.31         | 0/303   | 0.79        | 0/397         |
| 31  | G     | 0.29         | 0/1788  | 0.88        | 2/2408 (0.1%) |
| 32  | H     | 0.32         | 0/1652  | 0.90        | 3/2225 (0.1%) |



| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 33  | I     | 0.29         | 0/1665   | 0.87        | 3/2227 (0.1%)     |
| 34  | J     | 0.31         | 0/1170   | 1.01        | 10/1573 (0.6%)    |
| 35  | K     | 0.32         | 0/836    | 1.03        | 7/1128 (0.6%)     |
| 36  | L     | 0.30         | 0/1196   | 0.88        | 1/1602 (0.1%)     |
| 37  | M     | 0.30         | 0/989    | 0.92        | 2/1326 (0.2%)     |
| 38  | N     | 0.31         | 0/1034   | 0.93        | 3/1375 (0.2%)     |
| 39  | O     | 0.34         | 0/797    | 0.92        | 5/1077 (0.5%)     |
| 40  | P     | 0.32         | 0/886    | 0.94        | 3/1195 (0.3%)     |
| 41  | Q     | 0.30         | 0/969    | 0.99        | 5/1300 (0.4%)     |
| 42  | R     | 0.33         | 0/893    | 0.94        | 4/1193 (0.3%)     |
| 43  | S     | 0.29         | 0/817    | 0.88        | 1/1088 (0.1%)     |
| 44  | T     | 0.28         | 0/722    | 0.86        | 1/964 (0.1%)      |
| 45  | U     | 0.32         | 0/659    | 0.97        | 1/884 (0.1%)      |
| 46  | V     | 0.27         | 0/658    | 0.95        | 0/881             |
| 47  | W     | 0.32         | 0/545    | 0.90        | 1/731 (0.1%)      |
| 48  | X     | 0.32         | 0/653    | 0.89        | 1/877 (0.1%)      |
| 49  | Y     | 0.28         | 0/671    | 0.88        | 1/888 (0.1%)      |
| 50  | Z     | 0.33         | 0/551    | 1.02        | 5/728 (0.7%)      |
| 51  | a     | 0.31         | 0/1034   | 0.77        | 0/1387            |
| 52  | 3     | 0.41         | 0/36963  | 0.47        | 1/57662 (0.0%)    |
| 53  | 1     | 0.40         | 0/69796  | 0.48        | 4/108888 (0.0%)   |
| 54  | 2     | 0.41         | 0/2872   | 0.47        | 0/4479            |
| 55  | 5     | 0.41         | 0/1832   | 0.45        | 0/2855            |
| 55  | 6     | 0.42         | 0/1832   | 0.49        | 1/2855 (0.0%)     |
| 56  | 4     | 0.43         | 0/436    | 0.50        | 0/679             |
| 57  | 7     | 0.40         | 0/1809   | 0.48        | 0/2819            |
| 58  | 8     | 0.32         | 0/3084   | 0.91        | 9/4173 (0.2%)     |
| All | All   | 0.38         | 0/166283 | 0.62        | 145/248251 (0.1%) |

There are no bond length outliers.

All (145) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 45  | U     | 78  | VAL  | N-CA-C | -10.87 | 100.36      | 111.88   |
| 58  | 8     | 100 | ASP  | N-CA-C | -9.39  | 101.82      | 113.28   |
| 11  | l     | 95  | LEU  | N-CA-C | -7.95  | 103.04      | 112.89   |
| 41  | Q     | 114 | SER  | N-CA-C | -7.91  | 102.74      | 111.36   |
| 16  | q     | 49  | ARG  | N-CA-C | -7.71  | 102.96      | 113.30   |
| 34  | J     | 117 | ALA  | N-CA-C | -7.46  | 102.83      | 112.23   |
| 34  | J     | 101 | GLY  | N-CA-C | -7.45  | 102.90      | 115.34   |
| 7   | h     | 51  | TYR  | N-CA-C | 7.32   | 119.90      | 111.11   |
| 6   | g     | 10  | ALA  | N-CA-C | 7.28   | 120.13      | 111.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | h     | 43   | LYS  | N-CA-C      | -7.14 | 103.58      | 111.36   |
| 6   | g     | 67   | ALA  | N-CA-C      | -6.87 | 103.85      | 111.82   |
| 48  | X     | 57   | VAL  | N-CA-C      | 6.81  | 114.48      | 108.63   |
| 11  | l     | 114  | GLY  | N-CA-C      | 6.78  | 118.95      | 112.04   |
| 10  | k     | 71   | ARG  | N-CA-C      | -6.67 | 101.17      | 109.64   |
| 22  | w     | 52   | ASP  | N-CA-C      | -6.62 | 104.78      | 112.92   |
| 7   | h     | 117  | LEU  | N-CA-C      | 6.60  | 120.26      | 109.24   |
| 2   | c     | 98   | VAL  | N-CA-C      | -6.51 | 106.39      | 112.83   |
| 35  | K     | 90   | MET  | N-CA-C      | 6.47  | 117.99      | 108.86   |
| 18  | s     | 91   | GLY  | N-CA-C      | 6.46  | 122.77      | 115.08   |
| 10  | k     | 68   | GLY  | N-CA-C      | 6.46  | 120.82      | 112.68   |
| 34  | J     | 82   | HIS  | N-CA-C      | 6.42  | 113.78      | 108.07   |
| 6   | g     | 30   | LEU  | N-CA-C      | 6.41  | 118.35      | 111.36   |
| 39  | O     | 60   | ASP  | N-CA-C      | 6.41  | 118.26      | 111.28   |
| 13  | n     | 119  | SER  | N-CA-C      | -6.36 | 104.78      | 113.30   |
| 15  | p     | 22   | GLY  | N-CA-C      | -6.36 | 106.92      | 114.48   |
| 10  | k     | 33   | ALA  | N-CA-C      | -6.35 | 100.57      | 110.42   |
| 34  | J     | 122  | VAL  | N-CA-C      | 6.32  | 122.47      | 109.34   |
| 58  | 8     | 299  | ILE  | N-CA-C      | 6.32  | 117.01      | 108.17   |
| 38  | N     | 62   | LEU  | N-CA-C      | 6.27  | 119.17      | 109.07   |
| 6   | g     | 72   | ILE  | N-CA-C      | -6.22 | 104.21      | 111.00   |
| 1   | b     | 87   | SER  | N-CA-C      | -6.20 | 105.67      | 113.72   |
| 12  | m     | 110  | GLU  | N-CA-C      | 6.20  | 118.55      | 111.11   |
| 1   | b     | 40   | GLY  | N-CA-C      | -6.18 | 106.79      | 115.32   |
| 1   | b     | 12   | ARG  | N-CA-C      | -6.17 | 106.07      | 113.97   |
| 58  | 8     | 99   | MET  | N-CA-C      | 6.17  | 118.69      | 109.25   |
| 10  | k     | 67   | LYS  | N-CA-C      | -6.10 | 105.49      | 113.12   |
| 20  | u     | 6    | ARG  | N-CA-C      | 6.08  | 118.44      | 111.02   |
| 41  | Q     | 54   | VAL  | N-CA-C      | 6.07  | 117.89      | 109.45   |
| 41  | Q     | 43   | LYS  | N-CA-C      | 6.06  | 123.20      | 109.81   |
| 50  | Z     | 29   | ALA  | N-CA-C      | -6.03 | 105.78      | 113.02   |
| 34  | J     | 87   | VAL  | N-CA-C      | 5.98  | 117.45      | 109.37   |
| 53  | 1     | 490  | C    | C2'-C3'-O3' | 5.91  | 118.36      | 109.50   |
| 53  | 1     | 1130 | U    | C2'-C3'-O3' | 5.88  | 118.32      | 109.50   |
| 34  | J     | 116  | VAL  | N-CA-C      | -5.87 | 105.03      | 113.07   |
| 39  | O     | 77   | VAL  | N-CA-C      | 5.85  | 118.41      | 111.09   |
| 40  | P     | 70   | ALA  | N-CA-C      | -5.83 | 105.00      | 111.36   |
| 13  | n     | 43   | GLU  | N-CA-C      | -5.83 | 106.79      | 114.31   |
| 42  | R     | 64   | VAL  | N-CA-C      | 5.79  | 115.89      | 108.82   |
| 20  | u     | 82   | VAL  | N-CA-C      | 5.79  | 118.27      | 109.12   |
| 6   | g     | 19   | VAL  | N-CA-C      | 5.73  | 116.47      | 109.30   |
| 3   | d     | 115  | GLN  | N-CA-C      | -5.72 | 105.64      | 113.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 50  | Z     | 21   | SER  | N-CA-C      | -5.70 | 105.43      | 112.90   |
| 53  | 1     | 1020 | A    | C2'-C3'-O3' | 5.70  | 118.05      | 109.50   |
| 32  | H     | 177  | LEU  | N-CA-C      | 5.69  | 119.03      | 111.75   |
| 31  | G     | 9    | LEU  | N-CA-C      | -5.69 | 106.18      | 113.23   |
| 42  | R     | 82   | LEU  | N-CA-C      | -5.69 | 105.45      | 112.90   |
| 37  | M     | 55   | LYS  | CA-C-N      | 5.67  | 126.93      | 119.84   |
| 37  | M     | 55   | LYS  | C-N-CA      | 5.67  | 126.93      | 119.84   |
| 18  | s     | 20   | VAL  | N-CA-C      | 5.66  | 116.44      | 110.72   |
| 1   | b     | 35   | LYS  | N-CA-C      | 5.66  | 118.44      | 109.96   |
| 35  | K     | 11   | HIS  | CA-C-N      | 5.66  | 126.91      | 119.84   |
| 35  | K     | 11   | HIS  | C-N-CA      | 5.66  | 126.91      | 119.84   |
| 38  | N     | 128  | LYS  | N-CA-C      | 5.66  | 117.12      | 111.07   |
| 7   | h     | 44   | ALA  | N-CA-C      | -5.62 | 105.30      | 111.82   |
| 58  | 8     | 361  | VAL  | N-CA-C      | 5.61  | 116.02      | 108.17   |
| 11  | l     | 98   | ALA  | N-CA-C      | -5.59 | 106.45      | 113.28   |
| 35  | K     | 27   | ALA  | N-CA-C      | -5.59 | 105.27      | 111.36   |
| 40  | P     | 125  | LYS  | N-CA-C      | 5.56  | 122.65      | 110.80   |
| 8   | i     | 24   | GLY  | CA-C-N      | 5.55  | 125.26      | 119.82   |
| 8   | i     | 24   | GLY  | C-N-CA      | 5.55  | 125.26      | 119.82   |
| 9   | j     | 44   | TYR  | N-CA-C      | 5.55  | 118.37      | 110.10   |
| 44  | T     | 43   | ALA  | N-CA-C      | -5.54 | 105.34      | 111.71   |
| 58  | 8     | 147  | LEU  | N-CA-C      | -5.53 | 105.33      | 111.36   |
| 42  | R     | 3    | ILE  | N-CA-C      | 5.51  | 115.80      | 107.80   |
| 49  | Y     | 6    | ALA  | N-CA-C      | -5.50 | 107.14      | 112.97   |
| 26  | B     | 9    | ARG  | N-CA-C      | -5.49 | 105.31      | 112.23   |
| 2   | c     | 71   | ALA  | N-CA-C      | -5.49 | 106.63      | 113.38   |
| 17  | r     | 43   | ASN  | N-CA-C      | -5.48 | 105.70      | 112.72   |
| 10  | k     | 92   | GLU  | N-CA-C      | -5.48 | 104.15      | 112.04   |
| 58  | 8     | 211  | PHE  | N-CA-C      | 5.48  | 118.29      | 110.24   |
| 13  | n     | 67   | PHE  | N-CA-C      | -5.47 | 107.26      | 114.04   |
| 12  | m     | 13   | HIS  | N-CA-C      | 5.46  | 117.58      | 110.43   |
| 41  | Q     | 108  | ASP  | N-CA-C      | 5.46  | 117.29      | 110.91   |
| 50  | Z     | 49   | ALA  | N-CA-C      | -5.43 | 105.44      | 111.36   |
| 24  | y     | 14   | LEU  | N-CA-C      | -5.43 | 105.44      | 111.36   |
| 47  | W     | 66   | LEU  | N-CA-C      | -5.41 | 106.84      | 113.50   |
| 7   | h     | 100  | ALA  | N-CA-C      | -5.41 | 105.42      | 112.23   |
| 34  | J     | 144  | GLU  | N-CA-C      | -5.40 | 105.43      | 112.23   |
| 17  | r     | 49   | ILE  | N-CA-C      | 5.36  | 115.61      | 108.11   |
| 35  | K     | 38   | ARG  | N-CA-C      | 5.33  | 116.75      | 109.18   |
| 14  | o     | 78   | VAL  | N-CA-C      | 5.33  | 115.53      | 110.42   |
| 41  | Q     | 23   | LEU  | N-CA-C      | -5.33 | 104.09      | 111.28   |
| 11  | l     | 115  | GLU  | N-CA-C      | 5.31  | 117.12      | 110.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | r     | 50   | GLY  | N-CA-C      | -5.31 | 100.60      | 113.18   |
| 4   | e     | 106  | ALA  | N-CA-C      | 5.30  | 116.75      | 110.97   |
| 34  | J     | 141  | ASP  | N-CA-C      | -5.29 | 105.18      | 111.69   |
| 1   | b     | 157  | ALA  | N-CA-C      | 5.29  | 118.14      | 110.42   |
| 40  | P     | 75   | GLU  | N-CA-C      | -5.26 | 106.36      | 112.89   |
| 9   | j     | 43   | GLU  | N-CA-C      | -5.25 | 104.89      | 113.19   |
| 38  | N     | 6    | TYR  | N-CA-C      | 5.25  | 118.13      | 109.72   |
| 1   | b     | 131  | MET  | N-CA-C      | 5.25  | 119.25      | 113.21   |
| 13  | n     | 68   | ALA  | N-CA-C      | -5.25 | 105.98      | 112.38   |
| 17  | r     | 44   | GLY  | N-CA-C      | -5.25 | 100.75      | 113.18   |
| 16  | q     | 50   | ARG  | N-CA-C      | -5.24 | 107.55      | 114.31   |
| 4   | e     | 25   | MET  | N-CA-C      | -5.24 | 106.57      | 113.17   |
| 34  | J     | 123  | LEU  | N-CA-C      | -5.24 | 102.00      | 110.32   |
| 50  | Z     | 8    | ASN  | N-CA-C      | 5.23  | 121.95      | 110.80   |
| 52  | 3     | 1201 | A    | C2'-C3'-O3' | 5.22  | 117.33      | 109.50   |
| 18  | s     | 19   | LEU  | N-CA-C      | -5.21 | 105.51      | 111.14   |
| 36  | L     | 68   | VAL  | N-CA-C      | -5.21 | 108.20      | 113.20   |
| 3   | d     | 73   | ILE  | N-CA-C      | -5.20 | 106.82      | 112.80   |
| 33  | I     | 22   | SER  | N-CA-C      | -5.20 | 105.25      | 111.03   |
| 3   | d     | 139  | LYS  | N-CA-C      | -5.19 | 106.45      | 112.89   |
| 4   | e     | 105  | ILE  | N-CA-C      | 5.19  | 116.11      | 111.90   |
| 50  | Z     | 37   | TYR  | N-CA-C      | -5.19 | 107.31      | 113.38   |
| 13  | n     | 88   | ALA  | N-CA-C      | 5.17  | 116.60      | 110.97   |
| 10  | k     | 107  | LEU  | N-CA-C      | -5.15 | 106.95      | 113.18   |
| 1   | b     | 153  | LEU  | N-CA-C      | 5.14  | 118.09      | 110.48   |
| 32  | H     | 107  | LYS  | CA-C-N      | 5.14  | 124.64      | 119.19   |
| 32  | H     | 107  | LYS  | C-N-CA      | 5.14  | 124.64      | 119.19   |
| 58  | 8     | 23   | HIS  | N-CA-C      | -5.13 | 107.18      | 113.50   |
| 34  | J     | 134  | ASN  | N-CA-C      | 5.13  | 116.56      | 110.97   |
| 31  | G     | 45   | THR  | N-CA-C      | 5.13  | 116.68      | 111.14   |
| 13  | n     | 71   | ARG  | N-CA-C      | 5.12  | 121.71      | 110.80   |
| 1   | b     | 270  | ARG  | N-CA-C      | 5.12  | 117.89      | 110.42   |
| 16  | q     | 41   | ALA  | N-CA-C      | -5.11 | 106.31      | 112.54   |
| 1   | b     | 13   | ARG  | N-CA-C      | 5.11  | 117.51      | 111.33   |
| 33  | I     | 166  | LYS  | CA-C-N      | 5.10  | 126.22      | 119.84   |
| 33  | I     | 166  | LYS  | C-N-CA      | 5.10  | 126.22      | 119.84   |
| 35  | K     | 68   | GLN  | N-CA-C      | 5.10  | 117.58      | 111.71   |
| 7   | h     | 121  | SER  | N-CA-C      | 5.10  | 116.05      | 108.86   |
| 55  | 6     | 34   | C    | N1-C1'-C2'  | 5.08  | 119.62      | 112.00   |
| 39  | O     | 21   | ALA  | N-CA-C      | -5.08 | 105.83      | 112.23   |
| 58  | 8     | 191  | GLU  | N-CA-C      | -5.05 | 105.96      | 111.82   |
| 53  | 1     | 372  | G    | N9-C1'-C2'  | 5.05  | 119.58      | 112.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 58  | 8     | 316 | GLU  | N-CA-C | -5.04 | 108.16      | 114.56   |
| 7   | h     | 38  | MET  | N-CA-C | -5.04 | 106.91      | 113.16   |
| 20  | u     | 75  | ALA  | N-CA-C | -5.04 | 107.69      | 113.88   |
| 35  | K     | 66  | ALA  | N-CA-C | 5.03  | 113.92      | 108.14   |
| 42  | R     | 101 | THR  | N-CA-C | 5.03  | 119.47      | 113.23   |
| 39  | O     | 42  | LEU  | CA-C-N | 5.03  | 126.12      | 119.84   |
| 39  | O     | 42  | LEU  | C-N-CA | 5.03  | 126.12      | 119.84   |
| 27  | C     | 26  | LYS  | N-CA-C | 5.02  | 117.49      | 111.71   |
| 13  | n     | 48  | VAL  | N-CA-C | 5.01  | 115.24      | 110.53   |
| 43  | S     | 49  | THR  | N-CA-C | -5.01 | 106.43      | 112.54   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | b     | 2083  | 0        | 2157     | 66      | 0            |
| 2   | c     | 1565  | 0        | 1616     | 40      | 0            |
| 3   | d     | 1552  | 0        | 1619     | 34      | 0            |
| 4   | e     | 1411  | 0        | 1447     | 39      | 0            |
| 5   | f     | 1323  | 0        | 1374     | 30      | 0            |
| 6   | g     | 1111  | 0        | 1148     | 39      | 0            |
| 7   | h     | 989   | 0        | 1025     | 56      | 0            |
| 8   | i     | 1032  | 0        | 1088     | 35      | 0            |
| 9   | j     | 1129  | 0        | 1162     | 26      | 0            |
| 10  | k     | 939   | 0        | 1012     | 30      | 0            |
| 11  | l     | 1045  | 0        | 1117     | 32      | 0            |
| 12  | m     | 1074  | 0        | 1157     | 33      | 0            |
| 13  | n     | 961   | 0        | 1000     | 21      | 0            |
| 14  | o     | 892   | 0        | 923      | 23      | 0            |
| 15  | p     | 917   | 0        | 965      | 37      | 0            |
| 16  | q     | 947   | 0        | 1022     | 27      | 0            |
| 17  | r     | 816   | 0        | 839      | 24      | 0            |
| 18  | s     | 857   | 0        | 922      | 21      | 0            |
| 19  | t     | 739   | 0        | 807      | 22      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20  | u     | 780   | 0        | 834      | 17      | 0            |
| 21  | v     | 753   | 0        | 780      | 22      | 0            |
| 22  | w     | 575   | 0        | 592      | 12      | 0            |
| 23  | x     | 625   | 0        | 655      | 16      | 0            |
| 24  | y     | 509   | 0        | 543      | 22      | 0            |
| 25  | z     | 449   | 0        | 491      | 13      | 0            |
| 26  | B     | 444   | 0        | 461      | 12      | 0            |
| 27  | C     | 410   | 0        | 440      | 17      | 0            |
| 28  | D     | 377   | 0        | 418      | 18      | 0            |
| 29  | E     | 504   | 0        | 574      | 13      | 0            |
| 30  | F     | 302   | 0        | 343      | 24      | 0            |
| 31  | G     | 1757  | 0        | 1787     | 53      | 0            |
| 32  | H     | 1625  | 0        | 1699     | 68      | 0            |
| 33  | I     | 1643  | 0        | 1710     | 61      | 0            |
| 34  | J     | 1157  | 0        | 1199     | 40      | 0            |
| 35  | K     | 818   | 0        | 808      | 37      | 0            |
| 36  | L     | 1182  | 0        | 1240     | 36      | 0            |
| 37  | M     | 979   | 0        | 1034     | 31      | 0            |
| 38  | N     | 1022  | 0        | 1070     | 53      | 0            |
| 39  | O     | 787   | 0        | 828      | 40      | 0            |
| 40  | P     | 870   | 0        | 878      | 33      | 0            |
| 41  | Q     | 955   | 0        | 1019     | 39      | 0            |
| 42  | R     | 884   | 0        | 944      | 27      | 0            |
| 43  | S     | 805   | 0        | 847      | 35      | 0            |
| 44  | T     | 714   | 0        | 737      | 19      | 0            |
| 45  | U     | 649   | 0        | 666      | 25      | 0            |
| 46  | V     | 649   | 0        | 691      | 25      | 0            |
| 47  | W     | 536   | 0        | 552      | 15      | 0            |
| 48  | X     | 638   | 0        | 665      | 26      | 0            |
| 49  | Y     | 665   | 0        | 714      | 23      | 0            |
| 50  | Z     | 545   | 0        | 579      | 40      | 0            |
| 51  | a     | 1027  | 0        | 1092     | 39      | 0            |
| 52  | 3     | 33012 | 0        | 16618    | 556     | 0            |
| 53  | 1     | 62317 | 0        | 31346    | 909     | 0            |
| 54  | 2     | 2568  | 0        | 1303     | 48      | 0            |
| 55  | 5     | 1640  | 0        | 836      | 15      | 0            |
| 55  | 6     | 1640  | 0        | 837      | 29      | 0            |
| 56  | 4     | 388   | 0        | 196      | 2       | 0            |
| 57  | 7     | 1619  | 0        | 821      | 32      | 0            |
| 58  | 8     | 3028  | 0        | 3043     | 94      | 0            |
| 59  | 5     | 10    | 0        | 10       | 0       | 0            |
| 60  | 7     | 11    | 0        | 8        | 1       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61  | 8     | 32     | 0        | 12       | 1       | 0            |
| All | All   | 153282 | 0        | 104320   | 2874    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (2874) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:F:12:ARG:HH12  | 53:1:1102:C:H4'   | 1.23                     | 1.02              |
| 52:3:1259:C:H3'   | 52:3:1260:G:H5''  | 1.42                     | 1.01              |
| 38:N:114:LYS:NZ   | 52:3:1187:G:H5'   | 1.78                     | 0.98              |
| 10:k:48:PRO:HG3   | 52:3:1422:G:H5'   | 1.43                     | 0.97              |
| 53:1:1053:C:H2'   | 53:1:1054:A:H5''  | 1.47                     | 0.96              |
| 2:c:5:VAL:H       | 2:c:32:ASN:HD21   | 1.12                     | 0.96              |
| 53:1:1906:G:H2'   | 53:1:1907:G:H5''  | 1.47                     | 0.94              |
| 53:1:45:G:H5''    | 53:1:46:G:H5'     | 1.48                     | 0.93              |
| 10:k:121:GLU:HG3  | 10:k:122:VAL:HG23 | 1.52                     | 0.91              |
| 8:i:25:PRO:HG2    | 57:7:55:U:H3'     | 1.53                     | 0.90              |
| 57:7:7:A:H3'      | 57:7:8:U:H5''     | 1.54                     | 0.90              |
| 15:p:38:ARG:HE    | 52:3:345:C:H5'    | 1.34                     | 0.89              |
| 30:F:36:ARG:O     | 30:F:37:GLN:HB2   | 1.71                     | 0.89              |
| 38:N:46:VAL:HA    | 38:N:49:GLN:HG3   | 1.54                     | 0.89              |
| 7:h:116:GLU:HG3   | 7:h:117:LEU:HG    | 1.54                     | 0.88              |
| 12:m:12:MET:HA    | 53:1:910:A:H62    | 1.38                     | 0.88              |
| 54:2:13:G:H21     | 54:2:16:G:H1'     | 1.37                     | 0.88              |
| 53:1:906:U:H2'    | 53:1:907:G:H5''   | 1.55                     | 0.87              |
| 17:r:76:LYS:HB2   | 17:r:85:LYS:HB3   | 1.57                     | 0.86              |
| 53:1:2156:G:H2'   | 53:1:2157:G:H5'   | 1.55                     | 0.86              |
| 15:p:111:GLU:HB2  | 15:p:113:LEU:HD22 | 1.58                     | 0.86              |
| 43:S:50:LEU:HD12  | 43:S:51:PRO:HD2   | 1.57                     | 0.86              |
| 52:3:405:U:H3'    | 52:3:406:G:H5'    | 1.57                     | 0.86              |
| 37:M:28:SER:HB3   | 37:M:58:LEU:HB2   | 1.58                     | 0.86              |
| 42:R:97:ARG:HB2   | 42:R:99:GLN:HE22  | 1.39                     | 0.86              |
| 39:O:40:ILE:HB    | 39:O:73:LEU:HB3   | 1.58                     | 0.85              |
| 4:e:111:ARG:HD3   | 42:R:6:ILE:HG23   | 1.58                     | 0.85              |
| 57:7:25:C:H3'     | 57:7:26:A:H5''    | 1.58                     | 0.85              |
| 53:1:542:C:H2'    | 53:1:543:G:H5''   | 1.59                     | 0.85              |
| 53:1:1645:G:H5''  | 53:1:1646:C:H5'   | 1.57                     | 0.84              |
| 33:I:190:LEU:HD12 | 33:I:192:ALA:H    | 1.42                     | 0.84              |
| 52:3:960:U:H4'    | 52:3:961:U:O5'    | 1.77                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:2:3:C:H2'      | 54:2:4:C:H5''     | 1.60                     | 0.84              |
| 2:c:179:ARG:HB3   | 2:c:188:LEU:HD12  | 1.58                     | 0.83              |
| 1:b:106:PRO:HD2   | 1:b:109:LEU:HD22  | 1.61                     | 0.83              |
| 7:h:57:ASN:HB2    | 7:h:62:ARG:HD2    | 1.59                     | 0.82              |
| 28:D:12:ARG:HE    | 28:D:44:VAL:HG21  | 1.43                     | 0.82              |
| 42:R:64:VAL:HG22  | 42:R:65:GLU:H     | 1.42                     | 0.81              |
| 58:8:20:HIS:HB2   | 58:8:116:THR:HG22 | 1.62                     | 0.81              |
| 38:N:114:LYS:HZ2  | 52:3:1187:G:H5'   | 1.42                     | 0.81              |
| 37:M:12:ARG:NH2   | 52:3:826:C:H5'    | 1.94                     | 0.81              |
| 36:L:3:ARG:NH2    | 52:3:932:C:H5''   | 1.96                     | 0.80              |
| 33:I:120:LYS:HE2  | 33:I:130:ASN:HD21 | 1.45                     | 0.79              |
| 53:1:310:A:H2'    | 53:1:311:A:H5''   | 1.64                     | 0.79              |
| 32:H:156:LEU:HD11 | 32:H:163:ARG:HE   | 1.48                     | 0.79              |
| 24:y:2:LYS:HE2    | 53:1:102:U:H1'    | 1.64                     | 0.79              |
| 7:h:123:ILE:H     | 7:h:123:ILE:HD12  | 1.48                     | 0.79              |
| 53:1:1807:G:H2'   | 53:1:1808:A:H5'   | 1.65                     | 0.79              |
| 53:1:1906:G:C2'   | 53:1:1907:G:H5''  | 2.11                     | 0.79              |
| 53:1:1077:A:H2'   | 53:1:1078:U:H5'   | 1.64                     | 0.79              |
| 1:b:59:GLN:HA     | 53:1:1568:G:H5'   | 1.65                     | 0.79              |
| 7:h:3:LEU:HD23    | 7:h:5:LEU:H       | 1.47                     | 0.79              |
| 53:1:1133:A:H4'   | 53:1:1134:A:H5''  | 1.62                     | 0.78              |
| 53:1:215:G:H4'    | 53:1:216:A:H4'    | 1.64                     | 0.78              |
| 55:5:75:C:H2'     | 55:5:76:A:H5''    | 1.63                     | 0.78              |
| 53:1:1141:U:H4'   | 53:1:1142:A:O4'   | 1.83                     | 0.78              |
| 7:h:26:VAL:HB     | 7:h:82:ILE:HD11   | 1.66                     | 0.78              |
| 52:3:225:C:H2'    | 52:3:226:G:H5''   | 1.66                     | 0.78              |
| 17:r:14:VAL:HG21  | 17:r:98:ILE:HD12  | 1.66                     | 0.78              |
| 52:3:327:A:O2'    | 52:3:328:C:H4'    | 1.85                     | 0.77              |
| 31:G:30:ILE:HD11  | 31:G:38:HIS:HB3   | 1.66                     | 0.77              |
| 53:1:1020:A:H1'   | 53:1:1021:A:OP2   | 1.83                     | 0.77              |
| 1:b:153:LEU:HD13  | 1:b:175:LEU:HD21  | 1.67                     | 0.76              |
| 52:3:955:U:H3     | 52:3:1225:A:H61   | 1.31                     | 0.76              |
| 53:1:503:A:H4'    | 53:1:505:A:H5''   | 1.66                     | 0.76              |
| 53:1:2286:G:H5''  | 53:1:2287:A:OP1   | 1.86                     | 0.76              |
| 39:O:57:VAL:O     | 39:O:58:ASN:HB2   | 1.86                     | 0.76              |
| 58:8:374:ARG:HG3  | 58:8:388:VAL:HG12 | 1.68                     | 0.76              |
| 53:1:2156:G:C2'   | 53:1:2157:G:H5'   | 2.16                     | 0.76              |
| 38:N:114:LYS:HZ1  | 52:3:1187:G:H5'   | 1.50                     | 0.75              |
| 51:a:194:VAL:HA   | 51:a:197:LYS:HE2  | 1.67                     | 0.75              |
| 53:1:1801:A:H5''  | 53:1:2203:U:H2'   | 1.66                     | 0.75              |
| 45:U:46:LYS:HG3   | 45:U:47:GLU:H     | 1.52                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:3:279:A:H5'    | 52:3:281:G:H5'    | 1.68                     | 0.75              |
| 36:L:149:ALA:HB1  | 40:P:58:THR:HG21  | 1.69                     | 0.75              |
| 52:3:1346:A:H2'   | 52:3:1347:G:H4'   | 1.69                     | 0.75              |
| 32:H:122:GLN:HG3  | 32:H:127:VAL:HG11 | 1.68                     | 0.74              |
| 52:3:1197:A:H2'   | 52:3:1198:G:H5''  | 1.69                     | 0.74              |
| 32:H:34:SER:HA    | 32:H:37:LYS:HE3   | 1.70                     | 0.74              |
| 58:8:215:ILE:HD12 | 58:8:228:VAL:HG21 | 1.69                     | 0.74              |
| 53:1:580:U:H2'    | 53:1:581:C:C6     | 2.23                     | 0.74              |
| 3:d:163:ASN:HB2   | 53:1:322:A:OP2    | 1.87                     | 0.74              |
| 32:H:171:ARG:HG3  | 52:3:1106:G:H5''  | 1.70                     | 0.74              |
| 39:O:53:ILE:HG13  | 43:S:84:ARG:HD2   | 1.69                     | 0.74              |
| 52:3:1201:A:H1'   | 52:3:1202:U:OP2   | 1.87                     | 0.74              |
| 52:3:555:U:H2'    | 52:3:556:C:C6     | 2.23                     | 0.74              |
| 57:7:6:G:H3'      | 57:7:7:A:H5''     | 1.69                     | 0.73              |
| 53:1:310:A:C2'    | 53:1:311:A:H5''   | 2.17                     | 0.73              |
| 41:Q:39:THR:HG22  | 41:Q:40:THR:H     | 1.53                     | 0.73              |
| 51:a:53:ARG:HH12  | 51:a:168:ASN:HA   | 1.53                     | 0.73              |
| 36:L:142:ARG:HB3  | 55:6:41:C:H4'     | 1.70                     | 0.73              |
| 1:b:42:ARG:N      | 1:b:42:ARG:HD2    | 2.04                     | 0.73              |
| 8:i:118:GLY:HA2   | 53:1:1082:U:H5'   | 1.71                     | 0.72              |
| 17:r:35:PHE:HB2   | 17:r:59:ILE:HB    | 1.70                     | 0.72              |
| 29:E:61:LEU:HD12  | 29:E:61:LEU:O     | 1.88                     | 0.72              |
| 38:N:35:GLU:HA    | 38:N:39:GLY:HA3   | 1.71                     | 0.72              |
| 7:h:43:LYS:HA     | 7:h:46:ARG:HD2    | 1.72                     | 0.72              |
| 57:7:47:U:H2'     | 57:7:50:U:OP1     | 1.88                     | 0.72              |
| 2:c:148:GLN:HB2   | 2:c:152:PRO:HG2   | 1.72                     | 0.71              |
| 7:h:61:ARG:HB3    | 53:1:1046:A:H4'   | 1.71                     | 0.71              |
| 32:H:180:ASP:HB3  | 32:H:204:GLY:H    | 1.54                     | 0.71              |
| 39:O:50:THR:HG21  | 52:3:1367:C:H4'   | 1.71                     | 0.71              |
| 57:7:7:A:H3'      | 57:7:8:U:C5'      | 2.20                     | 0.71              |
| 29:E:31:ILE:O     | 29:E:31:ILE:HG13  | 1.89                     | 0.71              |
| 57:7:6:G:C3'      | 57:7:7:A:H5''     | 2.20                     | 0.71              |
| 30:F:24:ARG:NH2   | 30:F:36:ARG:HG3   | 2.05                     | 0.71              |
| 52:3:501:C:H2'    | 52:3:502:A:C8     | 2.25                     | 0.71              |
| 53:1:2134:A:N6    | 53:1:2157:G:H4'   | 2.06                     | 0.71              |
| 4:e:90:LEU:HD12   | 4:e:90:LEU:O      | 1.91                     | 0.71              |
| 41:Q:79:ILE:HG22  | 41:Q:103:CYS:HB3  | 1.71                     | 0.71              |
| 52:3:484:G:H4'    | 52:3:485:U:H5''   | 1.72                     | 0.71              |
| 1:b:146:LYS:HB2   | 1:b:149:LYS:HB2   | 1.71                     | 0.70              |
| 6:g:9:VAL:HB      | 6:g:13:GLY:HA3    | 1.72                     | 0.70              |
| 46:V:16:MET:HG3   | 46:V:19:SER:HB2   | 1.74                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:J:80:LEU:HD13  | 34:J:122:VAL:HG11 | 1.72                     | 0.70              |
| 53:1:275:C:H2'    | 53:1:276:U:H4'    | 1.72                     | 0.70              |
| 53:1:2427:C:H5''  | 53:1:2429:G:H5'   | 1.73                     | 0.69              |
| 28:D:34:ARG:HD2   | 28:D:39:ARG:HD2   | 1.72                     | 0.69              |
| 33:I:57:LYS:HD3   | 33:I:202:LEU:HD23 | 1.73                     | 0.69              |
| 52:3:367:U:H5'    | 58:8:280:ARG:HE   | 1.56                     | 0.69              |
| 8:i:20:SER:HB2    | 8:i:21:PRO:HD3    | 1.74                     | 0.69              |
| 53:1:704:G:H2'    | 53:1:726:G:N2     | 2.07                     | 0.69              |
| 2:c:56:LYS:HZ3    | 2:c:59:ARG:HB2    | 1.57                     | 0.69              |
| 34:J:107:GLY:H    | 34:J:110:MET:HE2  | 1.58                     | 0.69              |
| 53:1:2296:U:H5''  | 53:1:2297:A:OP1   | 1.91                     | 0.69              |
| 12:m:4:PRO:HG3    | 12:m:68:PHE:CE2   | 2.26                     | 0.69              |
| 53:1:1394:U:H4'   | 53:1:1603:A:H4'   | 1.73                     | 0.69              |
| 52:3:769:G:H4'    | 52:3:1513:A:H4'   | 1.73                     | 0.69              |
| 54:2:3:C:C2'      | 54:2:4:C:H5''     | 2.21                     | 0.69              |
| 1:b:106:PRO:HG2   | 1:b:109:LEU:HB2   | 1.73                     | 0.69              |
| 37:M:93:LYS:HE2   | 37:M:116:ARG:CZ   | 2.22                     | 0.69              |
| 32:H:192:TYR:HA   | 52:3:532:A:H61    | 1.57                     | 0.69              |
| 53:1:329:G:O4'    | 53:1:477:A:H1'    | 1.92                     | 0.69              |
| 50:Z:9:GLU:HB3    | 50:Z:10:PRO:HD3   | 1.74                     | 0.68              |
| 37:M:10:LEU:HD21  | 37:M:76:ARG:HB2   | 1.76                     | 0.68              |
| 39:O:50:THR:HG22  | 39:O:62:ARG:HD2   | 1.74                     | 0.68              |
| 39:O:57:VAL:HG22  | 39:O:58:ASN:H     | 1.58                     | 0.68              |
| 53:1:974:G:H1'    | 53:1:975:A:C8     | 2.28                     | 0.68              |
| 2:c:151:THR:HB    | 2:c:152:PRO:HD3   | 1.74                     | 0.68              |
| 5:f:163:TYR:HB2   | 5:f:166:GLU:HB2   | 1.75                     | 0.68              |
| 43:S:36:SER:HA    | 43:S:40:ARG:HD3   | 1.74                     | 0.68              |
| 50:Z:5:VAL:HG13   | 50:Z:19:LYS:NZ    | 2.08                     | 0.68              |
| 53:1:1367:A:H2'   | 53:1:1368:G:H5'   | 1.74                     | 0.68              |
| 35:K:50:PRO:HG3   | 35:K:55:HIS:HE1   | 1.58                     | 0.68              |
| 1:b:35:LYS:HB2    | 53:1:1570:A:H5'   | 1.76                     | 0.68              |
| 7:h:48:ALA:HB3    | 7:h:51:TYR:CE1    | 2.29                     | 0.68              |
| 20:u:47:PRO:HD3   | 20:u:55:GLY:HA2   | 1.74                     | 0.68              |
| 36:L:110:ARG:HH22 | 36:L:121:ASN:HD22 | 1.42                     | 0.68              |
| 43:S:2:LYS:HD2    | 52:3:1216:A:OP1   | 1.94                     | 0.68              |
| 48:X:77:ARG:HD2   | 52:3:1225:A:H1'   | 1.75                     | 0.68              |
| 53:1:2286:G:H4'   | 53:1:2287:A:O4'   | 1.94                     | 0.68              |
| 28:D:11:LYS:HE3   | 53:1:686:U:H5''   | 1.75                     | 0.68              |
| 40:P:126:ARG:HH21 | 52:3:692:U:H5''   | 1.57                     | 0.68              |
| 41:Q:23:LEU:HD13  | 41:Q:29:LYS:NZ    | 2.08                     | 0.68              |
| 55:5:75:C:C2'     | 55:5:76:A:H5''    | 2.24                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:H:198:LYS:HE3  | 52:3:1058:G:OP1   | 1.94                     | 0.68              |
| 39:O:45:ARG:HH22  | 52:3:1279:G:H8    | 1.41                     | 0.68              |
| 48:X:77:ARG:HH11  | 52:3:1222:G:H5''  | 1.58                     | 0.68              |
| 50:Z:50:SER:HA    | 50:Z:53:LYS:HE2   | 1.74                     | 0.68              |
| 53:1:2277:G:H2'   | 53:1:2278:A:H5''  | 1.76                     | 0.68              |
| 53:1:1053:C:C2'   | 53:1:1054:A:H5''  | 2.23                     | 0.68              |
| 55:6:17:C:H2'     | 55:6:17(A):U:C5   | 2.29                     | 0.68              |
| 49:Y:23:ARG:O     | 49:Y:26:MET:HG3   | 1.93                     | 0.67              |
| 55:5:6:G:O2'      | 55:5:7:G:H5'      | 1.93                     | 0.67              |
| 58:8:11:PRO:HD2   | 58:8:75:ARG:HA    | 1.77                     | 0.67              |
| 1:b:7:PRO:HB3     | 1:b:13:ARG:HG3    | 1.76                     | 0.67              |
| 18:s:59:GLU:HB3   | 18:s:66:ILE:HD11  | 1.75                     | 0.67              |
| 47:W:11:ARG:HB3   | 52:3:845:A:O2'    | 1.95                     | 0.67              |
| 53:1:546:U:H2'    | 53:1:547:A:H4'    | 1.76                     | 0.67              |
| 53:1:615:U:H5''   | 53:1:616:A:OP2    | 1.93                     | 0.67              |
| 53:1:906:U:C2'    | 53:1:907:G:H5''   | 2.24                     | 0.67              |
| 6:g:125:THR:HG23  | 6:g:146:VAL:O     | 1.94                     | 0.67              |
| 38:N:62:LEU:HB3   | 38:N:64:ILE:HD11  | 1.74                     | 0.67              |
| 42:R:100:ARG:HH12 | 52:3:950:U:H3'    | 1.59                     | 0.67              |
| 1:b:42:ARG:HH12   | 53:1:690:G:H21    | 1.41                     | 0.67              |
| 15:p:112:ARG:C    | 15:p:113:LEU:HD23 | 2.20                     | 0.67              |
| 51:a:206:GLY:H    | 53:1:1861:G:P     | 2.17                     | 0.67              |
| 52:3:501:C:H2'    | 52:3:502:A:H8     | 1.58                     | 0.67              |
| 6:g:58:LEU:O      | 6:g:61:VAL:HG22   | 1.94                     | 0.67              |
| 18:s:56:ALA:HA    | 18:s:59:GLU:HG2   | 1.75                     | 0.67              |
| 36:L:75:LYS:O     | 36:L:86:VAL:HG22  | 1.94                     | 0.67              |
| 52:3:946:A:H2'    | 52:3:947:G:C8     | 2.30                     | 0.67              |
| 53:1:2646:C:H2'   | 53:1:2647:U:O4'   | 1.93                     | 0.67              |
| 12:m:45:GLN:HE21  | 53:1:2485:G:H5''  | 1.59                     | 0.67              |
| 34:J:156:ARG:HH11 | 37:M:100:ILE:HG23 | 1.57                     | 0.67              |
| 53:1:2682:A:H61   | 53:1:2728:U:H1'   | 1.57                     | 0.67              |
| 2:c:149:ASN:HB3   | 53:1:2572:A:OP2   | 1.94                     | 0.67              |
| 15:p:31:VAL:HG23  | 15:p:38:ARG:HB3   | 1.77                     | 0.67              |
| 58:8:5:LYS:HD3    | 58:8:265:LEU:HB2  | 1.77                     | 0.67              |
| 49:Y:80:ALA:HA    | 49:Y:83:ASN:HD21  | 1.59                     | 0.67              |
| 12:m:3:GLN:HE21   | 12:m:92:TRP:HE1   | 1.42                     | 0.66              |
| 47:W:56:ARG:O     | 47:W:60:ARG:HG3   | 1.95                     | 0.66              |
| 52:3:1251:A:O2'   | 52:3:1370:G:H5'   | 1.95                     | 0.66              |
| 4:e:107:VAL:CG2   | 4:e:108:PRO:HD3   | 2.25                     | 0.66              |
| 22:w:39:THR:H     | 53:1:2331:G:H4'   | 1.60                     | 0.66              |
| 37:M:120:LEU:HB2  | 52:3:600:A:H5'    | 1.77                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:I:8:LEU:HD21   | 33:I:31:CYS:SG    | 2.35                     | 0.66              |
| 34:J:107:GLY:HA2  | 52:3:8:A:H1'      | 1.78                     | 0.66              |
| 36:L:41:ILE:HD11  | 52:3:1240:U:H5'   | 1.77                     | 0.66              |
| 46:V:18:LYS:HE3   | 52:3:255:G:H4'    | 1.78                     | 0.66              |
| 52:3:1429:A:H2'   | 52:3:1430:A:H8    | 1.60                     | 0.66              |
| 53:1:45:G:H5''    | 53:1:46:G:C5'     | 2.24                     | 0.66              |
| 57:7:62:C:H2'     | 57:7:63:G:O4'     | 1.94                     | 0.66              |
| 8:i:21:PRO:HB2    | 8:i:22:PRO:HD3    | 1.77                     | 0.66              |
| 10:k:47:ILE:HG13  | 10:k:48:PRO:HD2   | 1.77                     | 0.66              |
| 8:i:55:PRO:HD3    | 8:i:74:PRO:HD3    | 1.77                     | 0.66              |
| 18:s:42:LYS:HB2   | 53:1:2010:G:H5''  | 1.78                     | 0.66              |
| 29:E:18:LYS:HG2   | 53:1:651:G:H5'    | 1.78                     | 0.66              |
| 41:Q:69:GLU:HG3   | 52:3:521:G:H4'    | 1.76                     | 0.66              |
| 53:1:2553:G:H3'   | 53:1:2554:U:H5''  | 1.78                     | 0.66              |
| 55:6:17:C:H2'     | 55:6:17(A):U:H5   | 1.61                     | 0.66              |
| 2:c:156:PHE:HB3   | 9:j:81:ILE:HG22   | 1.78                     | 0.66              |
| 53:1:1386:C:H2'   | 53:1:1387:A:C8    | 2.31                     | 0.66              |
| 57:7:58:A:H1'     | 57:7:60:U:H5      | 1.60                     | 0.66              |
| 58:8:157:LEU:HD12 | 58:8:158:LEU:HD12 | 1.77                     | 0.66              |
| 58:8:215:ILE:HD11 | 58:8:293:LEU:HD23 | 1.78                     | 0.66              |
| 31:G:94:ARG:NH2   | 52:3:1100:C:H3'   | 2.11                     | 0.66              |
| 2:c:194:PRO:HA    | 53:1:2680:U:H5'   | 1.78                     | 0.65              |
| 4:e:73:VAL:HG12   | 4:e:75:GLY:H      | 1.61                     | 0.65              |
| 9:j:45:THR:HB     | 9:j:48:VAL:HG12   | 1.77                     | 0.65              |
| 18:s:20:VAL:HG21  | 18:s:43:ALA:HB3   | 1.76                     | 0.65              |
| 40:P:88:PRO:HG3   | 50:Z:28:LEU:HD23  | 1.77                     | 0.65              |
| 33:I:13:ARG:HA    | 33:I:37:PRO:HB3   | 1.76                     | 0.65              |
| 41:Q:51:VAL:HG22  | 41:Q:52:CYS:H     | 1.60                     | 0.65              |
| 53:1:807:U:H2'    | 53:1:808:G:H8     | 1.59                     | 0.65              |
| 48:X:35:ARG:HH12  | 48:X:76:THR:HG22  | 1.62                     | 0.65              |
| 58:8:121:LEU:HD13 | 58:8:312:LEU:HD21 | 1.79                     | 0.65              |
| 1:b:245:THR:OG1   | 1:b:249:VAL:HG12  | 1.97                     | 0.65              |
| 4:e:140:ILE:HG22  | 4:e:142:TYR:H     | 1.59                     | 0.65              |
| 33:I:28:ASP:HB2   | 33:I:31:CYS:SG    | 2.36                     | 0.65              |
| 45:U:4:ILE:HG12   | 45:U:21:VAL:HG12  | 1.77                     | 0.65              |
| 57:7:16:U:H1'     | 57:7:60:U:H1'     | 1.77                     | 0.65              |
| 6:g:66:ASN:HD22   | 6:g:135:HIS:HB2   | 1.62                     | 0.65              |
| 9:j:8:PRO:HG3     | 9:j:48:VAL:HG23   | 1.79                     | 0.65              |
| 13:n:63:ARG:HD2   | 53:1:1454:C:O4'   | 1.97                     | 0.65              |
| 53:1:473:G:O2'    | 53:1:474:G:H5'    | 1.97                     | 0.65              |
| 53:1:1825:U:H2'   | 53:1:1826:G:H8    | 1.62                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 43:S:17:ASP:C    | 43:S:22:LYS:HE3   | 2.22                     | 0.65              |
| 10:k:76:VAL:H    | 15:p:72:VAL:HG12  | 1.62                     | 0.65              |
| 28:D:12:ARG:NE   | 28:D:44:VAL:HG21  | 2.12                     | 0.65              |
| 52:3:17:U:H2'    | 52:3:18:C:C6      | 2.32                     | 0.65              |
| 53:1:1319:C:O2'  | 53:1:1320:C:H5'   | 1.95                     | 0.65              |
| 7:h:118:ILE:HG22 | 7:h:119:PRO:HD3   | 1.77                     | 0.65              |
| 12:m:45:GLN:NE2  | 53:1:2485:G:H5''  | 2.12                     | 0.65              |
| 19:t:11:LEU:HD11 | 19:t:32:LEU:HD13  | 1.78                     | 0.65              |
| 36:L:111:GLY:HA2 | 36:L:118:ARG:HD3  | 1.78                     | 0.65              |
| 53:1:1278:C:H2'  | 53:1:1279:G:H8    | 1.61                     | 0.65              |
| 9:j:7:LYS:HB2    | 9:j:10:THR:HG22   | 1.78                     | 0.64              |
| 14:o:75:GLY:HA3  | 14:o:109:ALA:HB3  | 1.79                     | 0.64              |
| 19:t:68:LYS:HD2  | 53:1:1336:A:OP2   | 1.97                     | 0.64              |
| 22:w:33:ILE:HG22 | 22:w:34:VAL:HG13  | 1.80                     | 0.64              |
| 52:3:1052:U:H2'  | 52:3:1200:C:H41   | 1.62                     | 0.64              |
| 58:8:137:LYS:HB3 | 58:8:140:MET:HE3  | 1.79                     | 0.64              |
| 5:f:174:LYS:O    | 5:f:175:LYS:HG2   | 1.96                     | 0.64              |
| 17:r:49:ILE:HD12 | 17:r:52:PRO:HA    | 1.80                     | 0.64              |
| 18:s:24:ILE:H    | 18:s:24:ILE:HD12  | 1.61                     | 0.64              |
| 55:6:50:U:H3     | 55:6:64:G:H1      | 1.44                     | 0.64              |
| 12:m:3:GLN:HE21  | 12:m:92:TRP:NE1   | 1.94                     | 0.64              |
| 13:n:51:LEU:HD11 | 13:n:70:THR:HG21  | 1.78                     | 0.64              |
| 48:X:24:SER:HB2  | 48:X:27:LYS:HE3   | 1.78                     | 0.64              |
| 52:3:664:G:H22   | 52:3:741:G:H1     | 1.43                     | 0.64              |
| 43:S:2:LYS:HE2   | 52:3:1048:G:H4'   | 1.80                     | 0.64              |
| 46:V:39:ARG:HD3  | 52:3:280:C:O2     | 1.98                     | 0.64              |
| 37:M:42:GLU:HG2  | 37:M:100:ILE:HD13 | 1.78                     | 0.64              |
| 52:3:355:C:H5'   | 52:3:355:C:H6     | 1.60                     | 0.64              |
| 53:1:2391:G:H2'  | 53:1:2424:C:H41   | 1.61                     | 0.64              |
| 32:H:155:ARG:C   | 32:H:156:LEU:HD23 | 2.23                     | 0.64              |
| 54:2:3:C:C3'     | 54:2:4:C:H5''     | 2.28                     | 0.64              |
| 11:l:110:VAL:HB  | 11:l:127:VAL:HG13 | 1.80                     | 0.64              |
| 31:G:111:LYS:O   | 31:G:114:LYS:HG2  | 1.98                     | 0.64              |
| 31:G:133:ALA:O   | 31:G:137:THR:HG23 | 1.98                     | 0.64              |
| 52:3:150:U:H3    | 52:3:171:A:H62    | 1.46                     | 0.64              |
| 30:F:12:ARG:NH1  | 53:1:1102:C:H4'   | 2.06                     | 0.64              |
| 32:H:112:ALA:HB3 | 32:H:184:ASN:HD22 | 1.62                     | 0.64              |
| 34:J:107:GLY:HA3 | 52:3:9:G:H5'      | 1.80                     | 0.64              |
| 52:3:730:G:H2'   | 52:3:731:G:H5'    | 1.80                     | 0.64              |
| 52:3:1513:A:H2'  | 52:3:1514:G:C8    | 2.33                     | 0.64              |
| 5:f:82:PHE:HB2   | 5:f:140:ILE:HD11  | 1.80                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:m:64:TRP:HB2   | 12:m:104:GLU:HB2  | 1.80                     | 0.64              |
| 35:K:66:ALA:HB1   | 35:K:67:PRO:HD2   | 1.80                     | 0.64              |
| 42:R:64:VAL:HG22  | 42:R:65:GLU:N     | 2.13                     | 0.64              |
| 49:Y:26:MET:HB3   | 52:3:1458:G:H5'   | 1.79                     | 0.64              |
| 51:a:5:THR:HG22   | 51:a:8:MET:HE3    | 1.80                     | 0.64              |
| 8:i:9:LYS:C       | 8:i:10:LEU:HD22   | 2.23                     | 0.63              |
| 14:o:84:GLU:OE2   | 14:o:85:LYS:HG2   | 1.98                     | 0.63              |
| 45:U:21:VAL:HG22  | 45:U:34:GLU:O     | 1.97                     | 0.63              |
| 52:3:29:U:O2'     | 52:3:30:U:H5'     | 1.99                     | 0.63              |
| 52:3:225:C:C2'    | 52:3:226:G:H5''   | 2.28                     | 0.63              |
| 58:8:205:ARG:HG2  | 58:8:272:GLY:HA3  | 1.80                     | 0.63              |
| 15:p:38:ARG:NE    | 52:3:345:C:H5'    | 2.09                     | 0.63              |
| 52:3:1352:C:H2'   | 52:3:1353:G:C8    | 2.34                     | 0.63              |
| 49:Y:67:HIS:HE1   | 52:3:132:C:H4'    | 1.62                     | 0.63              |
| 53:1:542:C:C2'    | 53:1:543:G:H5''   | 2.27                     | 0.63              |
| 58:8:90:LYS:NZ    | 58:8:337:ASP:HB2  | 2.13                     | 0.63              |
| 53:1:2039:U:H2'   | 53:1:2040:G:H8    | 1.63                     | 0.63              |
| 5:f:132:LEU:HD23  | 5:f:132:LEU:H     | 1.63                     | 0.63              |
| 53:1:2039:U:H2'   | 53:1:2040:G:C8    | 2.33                     | 0.63              |
| 2:c:118:PHE:CE1   | 2:c:163:GLY:HA2   | 2.34                     | 0.63              |
| 51:a:38:PHE:CD1   | 53:1:2127:G:H4'   | 2.34                     | 0.63              |
| 51:a:168:ASN:HD21 | 53:1:2179:C:H5'   | 1.62                     | 0.63              |
| 53:1:225:C:H2'    | 53:1:226:A:O4'    | 1.99                     | 0.63              |
| 53:1:995:C:H6     | 53:1:995:C:H5'    | 1.63                     | 0.63              |
| 34:J:133:ILE:O    | 34:J:136:VAL:HG12 | 1.99                     | 0.63              |
| 8:i:9:LYS:O       | 8:i:10:LEU:HD22   | 1.98                     | 0.63              |
| 50:Z:5:VAL:HG13   | 50:Z:19:LYS:HZ3   | 1.64                     | 0.63              |
| 52:3:1259:C:H3'   | 52:3:1260:G:C5'   | 2.23                     | 0.63              |
| 55:6:36:U:H2'     | 55:6:37:A:O4'     | 1.98                     | 0.63              |
| 57:7:9:A:O2'      | 57:7:46:G:H4'     | 1.98                     | 0.63              |
| 58:8:216:GLU:CD   | 58:8:230:GLY:HA2  | 2.23                     | 0.63              |
| 24:y:9:LYS:HZ2    | 24:y:11:VAL:HB    | 1.64                     | 0.62              |
| 45:U:31:ARG:HB2   | 52:3:310:G:H5''   | 1.81                     | 0.62              |
| 53:1:1071:G:OP1   | 53:1:1071:G:H3'   | 1.98                     | 0.62              |
| 6:g:51:ARG:HG2    | 6:g:55:GLU:CD     | 2.24                     | 0.62              |
| 40:P:121:ARG:HH21 | 50:Z:35:GLU:HG2   | 1.64                     | 0.62              |
| 53:1:2391:G:H2'   | 53:1:2424:C:N4    | 2.15                     | 0.62              |
| 53:1:2698:U:H2'   | 53:1:2699:C:C6    | 2.34                     | 0.62              |
| 8:i:42:ASN:HA     | 8:i:45:THR:HG22   | 1.80                     | 0.62              |
| 53:1:523:C:H2'    | 53:1:524:G:H8     | 1.63                     | 0.62              |
| 44:T:78:THR:O     | 44:T:82:GLU:HG3   | 1.98                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:435:C:H2'    | 53:1:436:C:H5'    | 1.81                     | 0.62              |
| 54:2:95:U:H2'     | 54:2:96:G:H8      | 1.64                     | 0.62              |
| 35:K:6:ILE:HB     | 35:K:62:MET:HB2   | 1.81                     | 0.62              |
| 35:K:50:PRO:HG3   | 35:K:55:HIS:CE1   | 2.35                     | 0.62              |
| 9:j:26:GLY:HA3    | 53:1:1140:C:H5'   | 1.80                     | 0.62              |
| 31:G:119:GLN:HE22 | 31:G:136:ARG:HH11 | 1.47                     | 0.62              |
| 36:L:3:ARG:HH22   | 52:3:932:C:H5''   | 1.64                     | 0.62              |
| 38:N:119:LYS:HG3  | 52:3:1349:A:OP1   | 2.00                     | 0.62              |
| 52:3:1137:C:H4'   | 52:3:1138:G:N2    | 2.14                     | 0.62              |
| 53:1:859:G:H1'    | 53:1:860:U:H5     | 1.65                     | 0.62              |
| 52:3:245:U:O2'    | 52:3:246:A:H5'    | 1.98                     | 0.62              |
| 58:8:309:VAL:HG11 | 58:8:359:MET:HE1  | 1.81                     | 0.62              |
| 15:p:113:LEU:HD11 | 52:3:1441:A:N1    | 2.15                     | 0.62              |
| 33:I:131:ILE:HG22 | 33:I:133:SER:H    | 1.64                     | 0.62              |
| 50:Z:19:LYS:HB3   | 50:Z:24:LYS:HD2   | 1.82                     | 0.62              |
| 6:g:132:PHE:HB2   | 6:g:140:ALA:HB3   | 1.82                     | 0.62              |
| 16:q:5:ARG:NH1    | 53:1:585:G:N7     | 2.47                     | 0.62              |
| 25:z:10:ARG:HB2   | 25:z:10:ARG:NH2   | 2.15                     | 0.62              |
| 31:G:169:HIS:O    | 31:G:173:LYS:HD3  | 1.99                     | 0.62              |
| 39:O:44:THR:HG22  | 39:O:70:HIS:HA    | 1.80                     | 0.62              |
| 42:R:23:GLY:HA2   | 42:R:68:LEU:HD22  | 1.81                     | 0.62              |
| 48:X:9:PHE:CD2    | 52:3:1318:A:H4'   | 2.35                     | 0.62              |
| 53:1:1300:G:H4'   | 53:1:1301:A:H5''  | 1.82                     | 0.62              |
| 53:1:1825:U:H2'   | 53:1:1826:G:C8    | 2.35                     | 0.62              |
| 1:b:7:PRO:O       | 53:1:1695:G:H1'   | 1.99                     | 0.61              |
| 29:E:2:LYS:HG3    | 53:1:242:G:C8     | 2.35                     | 0.61              |
| 10:k:104:THR:HG22 | 10:k:106:GLU:H    | 1.65                     | 0.61              |
| 18:s:85:ILE:HD12  | 18:s:85:ILE:N     | 2.15                     | 0.61              |
| 49:Y:43:LYS:HE2   | 49:Y:82:ILE:HB    | 1.82                     | 0.61              |
| 58:8:121:LEU:HD23 | 58:8:124:ARG:HH12 | 1.64                     | 0.61              |
| 16:q:18:LYS:O     | 16:q:18:LYS:HD3   | 1.99                     | 0.61              |
| 53:1:1077:A:C2'   | 53:1:1078:U:H5'   | 2.29                     | 0.61              |
| 35:K:23:GLU:HA    | 35:K:26:THR:HG22  | 1.81                     | 0.61              |
| 52:3:372:C:H41    | 52:3:387:U:H2'    | 1.66                     | 0.61              |
| 18:s:82:MET:HB2   | 18:s:98:LYS:HB2   | 1.81                     | 0.61              |
| 33:I:131:ILE:H    | 33:I:131:ILE:HD12 | 1.65                     | 0.61              |
| 53:1:639:U:H2'    | 53:1:640:C:C6     | 2.36                     | 0.61              |
| 1:b:224:MET:HE2   | 53:1:782:A:N1     | 2.15                     | 0.61              |
| 1:b:250:GLN:NE2   | 1:b:251:THR:O     | 2.33                     | 0.61              |
| 8:i:9:LYS:NZ      | 53:1:1070:A:N3    | 2.48                     | 0.61              |
| 12:m:75:GLU:HB3   | 12:m:90:GLU:HG3   | 1.82                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 37:M:12:ARG:CZ   | 52:3:826:C:H5'    | 2.30                     | 0.61              |
| 7:h:50:VAL:HG13  | 53:1:1083:U:OP2   | 2.00                     | 0.61              |
| 52:3:784:A:H4'   | 53:1:1837:C:OP1   | 2.01                     | 0.61              |
| 53:1:1991:U:H2'  | 53:1:1992:G:H5''  | 1.83                     | 0.61              |
| 21:v:16:ALA:HA   | 21:v:19:ARG:NH1   | 2.16                     | 0.61              |
| 34:J:76:ASN:HB2  | 34:J:81:GLN:NE2   | 2.16                     | 0.61              |
| 52:3:1238:A:H62  | 52:3:1301:U:H3    | 1.47                     | 0.61              |
| 19:t:15:HIS:H    | 19:t:32:LEU:HA    | 1.65                     | 0.61              |
| 31:G:45:THR:HG22 | 31:G:200:PRO:HB2  | 1.83                     | 0.61              |
| 53:1:807:U:H2'   | 53:1:808:G:C8     | 2.35                     | 0.61              |
| 58:8:144:GLU:HA  | 58:8:147:LEU:HB2  | 1.83                     | 0.61              |
| 6:g:51:ARG:HG2   | 6:g:55:GLU:OE2    | 2.01                     | 0.60              |
| 50:Z:13:VAL:HG13 | 50:Z:15:LEU:HG    | 1.83                     | 0.60              |
| 52:3:950:U:H2'   | 52:3:951:G:H8     | 1.66                     | 0.60              |
| 28:D:24:THR:HG23 | 28:D:27:GLY:H     | 1.66                     | 0.60              |
| 41:Q:50:LYS:HB3  | 41:Q:66:ILE:HB    | 1.82                     | 0.60              |
| 52:3:1137:C:H5'  | 52:3:1138:G:H5'   | 1.83                     | 0.60              |
| 53:1:1909:C:H2'  | 53:1:1910:G:H8    | 1.66                     | 0.60              |
| 17:r:65:ALA:HB3  | 17:r:95:ASP:HB3   | 1.82                     | 0.60              |
| 21:v:16:ALA:HA   | 21:v:19:ARG:HH12  | 1.65                     | 0.60              |
| 32:H:13:ILE:HG22 | 32:H:14:VAL:HG13  | 1.83                     | 0.60              |
| 45:U:12:LYS:O    | 45:U:13:LYS:HB2   | 2.02                     | 0.60              |
| 52:3:335:C:H2'   | 52:3:336:A:H8     | 1.67                     | 0.60              |
| 53:1:121:G:H4'   | 53:1:149:A:H5'    | 1.83                     | 0.60              |
| 53:1:1186:G:H2'  | 53:1:1187:G:O4'   | 2.01                     | 0.60              |
| 12:m:41:LEU:HD13 | 12:m:96:ILE:HG13  | 1.82                     | 0.60              |
| 11:l:3:LEU:HD23  | 53:1:1203:U:H4'   | 1.83                     | 0.60              |
| 52:3:784:A:H2'   | 52:3:785:G:C8     | 2.36                     | 0.60              |
| 53:1:704:G:H1'   | 53:1:727:A:H61    | 1.67                     | 0.60              |
| 53:1:1019:U:H3   | 53:1:1142:A:H62   | 1.48                     | 0.60              |
| 32:H:57:GLU:HB2  | 32:H:64:ARG:HB3   | 1.84                     | 0.60              |
| 12:m:4:PRO:HG2   | 12:m:70:ASP:HA    | 1.84                     | 0.60              |
| 39:O:49:PHE:HB2  | 39:O:65:TYR:HB2   | 1.83                     | 0.60              |
| 13:n:44:LEU:HD23 | 13:n:113:ILE:HD13 | 1.83                     | 0.60              |
| 37:M:54:THR:O    | 37:M:56:PRO:HD3   | 2.02                     | 0.60              |
| 52:3:225:C:C3'   | 52:3:226:G:H5''   | 2.32                     | 0.60              |
| 27:C:28:THR:HG23 | 27:C:29:LYS:HG2   | 1.83                     | 0.60              |
| 29:E:61:LEU:HD13 | 29:E:64:ALA:HB3   | 1.84                     | 0.60              |
| 52:3:634:C:H2'   | 52:3:635:A:H8     | 1.66                     | 0.60              |
| 37:M:91:LEU:HD12 | 37:M:92:PRO:HD2   | 1.83                     | 0.60              |
| 58:8:302:HIS:HB2 | 58:8:369:MET:HE2  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:G:160:LEU:HB2 | 31:G:182:VAL:HG12 | 1.82                     | 0.59              |
| 38:N:109:GLN:OE1 | 52:3:1116:U:H4'   | 2.02                     | 0.59              |
| 52:3:1414:U:H2'  | 52:3:1415:G:H8    | 1.65                     | 0.59              |
| 53:1:2800:A:H3'  | 53:1:2801:G:H5'   | 1.83                     | 0.59              |
| 33:I:50:TYR:CD2  | 52:3:508:U:H4'    | 2.36                     | 0.59              |
| 52:3:358:U:H2'   | 52:3:359:G:H8     | 1.67                     | 0.59              |
| 13:n:39:PRO:HG2  | 53:1:1651:G:H4'   | 1.84                     | 0.59              |
| 41:Q:48:LEU:HB2  | 52:3:520:A:OP1    | 2.02                     | 0.59              |
| 42:R:68:LEU:O    | 42:R:71:GLU:HG3   | 2.02                     | 0.59              |
| 3:d:131:THR:HG22 | 3:d:160:ALA:HA    | 1.84                     | 0.59              |
| 15:p:31:VAL:HG11 | 15:p:40:GLN:HE21  | 1.68                     | 0.59              |
| 53:1:2853:C:H2'  | 53:1:2854:G:C8    | 2.38                     | 0.59              |
| 2:c:155:VAL:HG21 | 53:1:2618:G:H21   | 1.67                     | 0.59              |
| 31:G:117:GLU:O   | 31:G:121:GLN:HG2  | 2.03                     | 0.59              |
| 32:H:55:VAL:HB   | 32:H:66:THR:HB    | 1.84                     | 0.59              |
| 52:3:1497:G:O2'  | 52:3:1498:U:H5'   | 2.03                     | 0.59              |
| 53:1:2512:C:H2'  | 53:1:2513:A:O4'   | 2.02                     | 0.59              |
| 57:7:51:U:H2'    | 57:7:52:G:C8      | 2.37                     | 0.59              |
| 57:7:53:G:H5''   | 58:8:321:THR:OG1  | 2.02                     | 0.59              |
| 41:Q:73:LEU:HD21 | 41:Q:79:ILE:HG21  | 1.85                     | 0.59              |
| 42:R:79:LEU:HD12 | 42:R:82:LEU:HD12  | 1.83                     | 0.59              |
| 43:S:68:ARG:NH1  | 52:3:1202:U:H5'   | 2.17                     | 0.59              |
| 52:3:1170:A:H2'  | 52:3:1171:A:O4'   | 2.02                     | 0.59              |
| 15:p:2:ASN:O     | 15:p:6:GLN:HG3    | 2.02                     | 0.59              |
| 22:w:34:VAL:O    | 22:w:54:THR:HG23  | 2.03                     | 0.59              |
| 28:D:34:ARG:NH2  | 53:1:466:A:OP1    | 2.35                     | 0.59              |
| 40:P:86:LYS:HB2  | 40:P:112:VAL:HG23 | 1.83                     | 0.59              |
| 44:T:50:HIS:CE1  | 52:3:667:G:H4'    | 2.38                     | 0.59              |
| 52:3:876:C:H2'   | 52:3:877:G:H8     | 1.68                     | 0.59              |
| 52:3:1105:A:H2'  | 52:3:1106:G:H8    | 1.68                     | 0.59              |
| 52:3:1354:U:H2'  | 52:3:1355:G:H8    | 1.67                     | 0.59              |
| 53:1:821:A:H5''  | 53:1:822:G:C5'    | 2.31                     | 0.59              |
| 53:1:2086:U:H2'  | 53:1:2087:G:C8    | 2.37                     | 0.59              |
| 53:1:2423:U:O2'  | 53:1:2425:A:H2'   | 2.01                     | 0.59              |
| 53:1:577:G:H2'   | 53:1:578:G:C8     | 2.38                     | 0.59              |
| 53:1:1810:A:H2'  | 53:1:1811:G:O4'   | 2.02                     | 0.59              |
| 15:p:96:LEU:HB3  | 15:p:99:LEU:HD13  | 1.85                     | 0.59              |
| 53:1:1251:C:O2'  | 53:1:1252:G:H3'   | 2.02                     | 0.59              |
| 55:6:54:U:H3     | 55:6:58:A:H62     | 1.51                     | 0.59              |
| 4:e:130:GLY:HA2  | 4:e:152:ASP:HA    | 1.85                     | 0.58              |
| 9:j:7:LYS:HG2    | 53:1:538:A:H4'    | 1.83                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:m:38:ARG:HG3   | 12:m:98:PRO:HD3   | 1.85                     | 0.58              |
| 24:y:41:HIS:CD2   | 53:1:96:C:H4'     | 2.37                     | 0.58              |
| 32:H:155:ARG:NH1  | 32:H:192:TYR:O    | 2.36                     | 0.58              |
| 38:N:91:GLU:HA    | 38:N:94:ARG:HB2   | 1.84                     | 0.58              |
| 53:1:2287:A:O2'   | 53:1:2288:A:H2'   | 2.02                     | 0.58              |
| 53:1:2834:G:H2'   | 53:1:2879:A:H61   | 1.67                     | 0.58              |
| 20:u:51:LEU:HD23  | 20:u:51:LEU:O     | 2.03                     | 0.58              |
| 51:a:11:ILE:HG23  | 51:a:33:LEU:HD22  | 1.84                     | 0.58              |
| 52:3:701:U:H4'    | 52:3:703:G:H1'    | 1.85                     | 0.58              |
| 52:3:880:C:H2'    | 52:3:881:G:H8     | 1.68                     | 0.58              |
| 52:3:1339:A:H2'   | 52:3:1340:A:H5'   | 1.85                     | 0.58              |
| 52:3:1413:A:H2    | 52:3:1487:G:H22   | 1.49                     | 0.58              |
| 10:k:109:SER:O    | 10:k:110:GLU:HG3  | 2.03                     | 0.58              |
| 31:G:137:THR:O    | 31:G:141:GLU:HG2  | 2.03                     | 0.58              |
| 52:3:367:U:H5'    | 58:8:280:ARG:NE   | 2.18                     | 0.58              |
| 52:3:1379:G:O2'   | 52:3:1380:U:H5'   | 2.02                     | 0.58              |
| 53:1:1300:G:H4'   | 53:1:1301:A:C5'   | 2.32                     | 0.58              |
| 54:2:95:U:H2'     | 54:2:96:G:C8      | 2.38                     | 0.58              |
| 11:l:19:LEU:HB2   | 53:1:587:C:O2'    | 2.04                     | 0.58              |
| 18:s:24:ILE:HG22  | 18:s:71:VAL:HG21  | 1.84                     | 0.58              |
| 52:3:1218:C:H2'   | 52:3:1219:A:C8    | 2.38                     | 0.58              |
| 53:1:49:A:H5'     | 53:1:51:G:O4'     | 2.02                     | 0.58              |
| 53:1:2799:A:H2'   | 53:1:2800:A:H5'   | 1.86                     | 0.58              |
| 58:8:83:PRO:HG3   | 58:8:91:ASN:HB2   | 1.86                     | 0.58              |
| 12:m:57:VAL:O     | 12:m:58:LYS:HG2   | 2.02                     | 0.58              |
| 17:r:78:ARG:HH12  | 53:1:990:A:H61    | 1.51                     | 0.58              |
| 32:H:178:ARG:HH21 | 52:3:1112:C:H4'   | 1.67                     | 0.58              |
| 53:1:703:U:H2'    | 53:1:704:G:O4'    | 2.03                     | 0.58              |
| 58:8:157:LEU:CD1  | 58:8:158:LEU:HD12 | 2.33                     | 0.58              |
| 12:m:69:PRO:HA    | 12:m:94:ALA:HB2   | 1.86                     | 0.58              |
| 52:3:946:A:H2'    | 52:3:947:G:H8     | 1.67                     | 0.58              |
| 57:7:50:U:H3      | 57:7:64:A:H61     | 1.49                     | 0.58              |
| 7:h:96:PHE:HE2    | 7:h:126:LEU:H     | 1.50                     | 0.58              |
| 39:O:59:LYS:HB2   | 52:3:972:C:H4'    | 1.85                     | 0.58              |
| 47:W:31:TYR:CG    | 47:W:54:LEU:HD11  | 2.39                     | 0.58              |
| 52:3:78:A:H2'     | 52:3:79:G:O4'     | 2.03                     | 0.58              |
| 52:3:1033:G:H2'   | 52:3:1034:G:H5''  | 1.86                     | 0.58              |
| 53:1:833:A:H2'    | 53:1:834:G:C8     | 2.39                     | 0.58              |
| 53:1:1278:C:H2'   | 53:1:1279:G:C8    | 2.39                     | 0.58              |
| 2:c:13:ARG:HH11   | 15:p:54:LEU:HD23  | 1.69                     | 0.58              |
| 36:L:49:LEU:HD22  | 36:L:123:LEU:HD23 | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:598:U:H2'    | 53:1:599:A:C8     | 2.38                     | 0.58              |
| 53:1:729:G:H4'    | 53:1:763:G:H5'    | 1.85                     | 0.58              |
| 53:1:833:A:H2'    | 53:1:834:G:H8     | 1.68                     | 0.58              |
| 55:5:75:C:C3'     | 55:5:76:A:H5''    | 2.34                     | 0.58              |
| 5:f:173:ALA:O     | 5:f:174:LYS:HG2   | 2.04                     | 0.58              |
| 26:B:28:SER:HB2   | 53:1:2885:G:O6    | 2.04                     | 0.58              |
| 39:O:6:ILE:HB     | 39:O:76:ILE:HB    | 1.84                     | 0.58              |
| 52:3:572:A:H5''   | 52:3:917:G:H4'    | 1.86                     | 0.58              |
| 53:1:1796:U:H2'   | 53:1:1797:G:H8    | 1.68                     | 0.58              |
| 53:1:2538:C:H2'   | 53:1:2539:C:H6    | 1.68                     | 0.58              |
| 53:1:2799:A:C2'   | 53:1:2800:A:H5'   | 2.33                     | 0.58              |
| 33:I:63:ILE:O     | 33:I:110:ARG:HD2  | 2.04                     | 0.57              |
| 53:1:858:G:H5'    | 53:1:859:G:OP2    | 2.04                     | 0.57              |
| 53:1:1067:A:H2'   | 53:1:1067:A:N3    | 2.19                     | 0.57              |
| 58:8:85:HIS:HB2   | 58:8:88:TYR:HB2   | 1.86                     | 0.57              |
| 11:l:122:VAL:HG21 | 11:l:135:ILE:HD13 | 1.86                     | 0.57              |
| 17:r:28:ALA:HB3   | 17:r:31:GLU:HB2   | 1.87                     | 0.57              |
| 52:3:1060:U:H3    | 52:3:1197:A:H61   | 1.50                     | 0.57              |
| 52:3:1158:C:H2'   | 52:3:1159:U:H4'   | 1.85                     | 0.57              |
| 53:1:466:A:H2'    | 53:1:467:G:H5'    | 1.86                     | 0.57              |
| 5:f:154:GLU:HG2   | 5:f:156:TYR:H     | 1.68                     | 0.57              |
| 53:1:1380:G:H1'   | 53:1:1569:A:H61   | 1.69                     | 0.57              |
| 53:1:2114:A:H61   | 53:1:2117:A:H62   | 1.52                     | 0.57              |
| 32:H:50:SER:HB2   | 32:H:114:LEU:HD11 | 1.87                     | 0.57              |
| 33:I:187:ARG:HD2  | 33:I:190:LEU:HD21 | 1.85                     | 0.57              |
| 52:3:1258:G:H2'   | 52:3:1259:C:C6    | 2.40                     | 0.57              |
| 52:3:1342:C:H2'   | 52:3:1343:G:H8    | 1.69                     | 0.57              |
| 52:3:1441:A:H2'   | 52:3:1442:G:H5'   | 1.85                     | 0.57              |
| 53:1:796:C:H2'    | 53:1:797:G:H8     | 1.68                     | 0.57              |
| 1:b:227:VAL:HG11  | 53:1:784:G:C6     | 2.40                     | 0.57              |
| 49:Y:67:HIS:CE1   | 52:3:132:C:H4'    | 2.39                     | 0.57              |
| 52:3:304:U:O2'    | 52:3:305:G:H5'    | 2.04                     | 0.57              |
| 53:1:1078:U:H4'   | 53:1:1079:C:H5''  | 1.85                     | 0.57              |
| 2:c:123:LYS:HZ1   | 53:1:2724:U:H5''  | 1.69                     | 0.57              |
| 5:f:174:LYS:HD3   | 53:1:2531:A:OP2   | 2.05                     | 0.57              |
| 18:s:24:ILE:HD11  | 18:s:36:LEU:HD21  | 1.87                     | 0.57              |
| 32:H:82:ASP:O     | 32:H:85:LYS:HG3   | 2.04                     | 0.57              |
| 39:O:41:PRO:HG3   | 52:3:1150:A:C2    | 2.39                     | 0.57              |
| 41:Q:23:LEU:HD22  | 41:Q:26:CYS:SG    | 2.44                     | 0.57              |
| 52:3:1256:A:H1'   | 52:3:1258:G:C4    | 2.39                     | 0.57              |
| 52:3:1412:C:H2'   | 52:3:1413:A:C8    | 2.39                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 58:8:90:LYS:HZ3  | 58:8:337:ASP:HB2 | 1.67                     | 0.57              |
| 1:b:153:LEU:HD13 | 1:b:175:LEU:CD2  | 2.35                     | 0.57              |
| 24:y:2:LYS:HG3   | 24:y:3:ALA:H     | 1.69                     | 0.57              |
| 25:z:8:GLN:HE22  | 25:z:23:LEU:HD13 | 1.70                     | 0.57              |
| 52:3:372:C:N4    | 52:3:387:U:H2'   | 2.20                     | 0.57              |
| 52:3:1256:A:H1'  | 52:3:1258:G:N9   | 2.20                     | 0.57              |
| 53:1:528:A:N1    | 53:1:2042:A:H2'  | 2.20                     | 0.57              |
| 53:1:2163:A:H2'  | 53:1:2164:C:H5'  | 1.86                     | 0.57              |
| 7:h:18:VAL:HA    | 7:h:86:MET:HE2   | 1.86                     | 0.57              |
| 7:h:31:ARG:HH21  | 53:1:1054:A:C4'  | 2.18                     | 0.57              |
| 53:1:1023:U:O2'  | 53:1:1122:G:H5'  | 2.05                     | 0.57              |
| 53:1:2432:A:H1'  | 55:6:75:C:H5'    | 1.87                     | 0.57              |
| 53:1:2547:A:H2'  | 53:1:2548:U:C6   | 2.40                     | 0.57              |
| 54:2:3:C:H3'     | 54:2:4:C:H5''    | 1.87                     | 0.57              |
| 58:8:314:LYS:HB2 | 58:8:320:HIS:HB3 | 1.87                     | 0.57              |
| 1:b:48:ILE:HD11  | 1:b:51:ARG:HA    | 1.86                     | 0.57              |
| 14:o:56:LYS:HA   | 14:o:59:ALA:HB3  | 1.86                     | 0.57              |
| 53:1:1524:G:H2'  | 53:1:1525:A:H8   | 1.69                     | 0.57              |
| 53:1:1697:G:H4'  | 53:1:1978:A:H5'' | 1.86                     | 0.57              |
| 53:1:2515:C:H2'  | 53:1:2516:A:H8   | 1.70                     | 0.57              |
| 58:8:53:ALA:HB3  | 58:8:56:GLU:HG3  | 1.87                     | 0.57              |
| 1:b:257:ARG:NH2  | 1:b:266:ILE:HD12 | 2.20                     | 0.57              |
| 35:K:68:GLN:O    | 35:K:71:ILE:HG22 | 2.05                     | 0.57              |
| 36:L:23:ALA:O    | 36:L:26:VAL:HG12 | 2.04                     | 0.57              |
| 37:M:9:MET:HG3   | 37:M:26:MET:SD   | 2.45                     | 0.57              |
| 41:Q:57:THR:HG21 | 52:3:363:A:OP2   | 2.05                     | 0.57              |
| 50:Z:48:LYS:HD3  | 52:3:723:U:H6    | 1.69                     | 0.57              |
| 53:1:69:C:O2'    | 53:1:70:G:H5'    | 2.05                     | 0.57              |
| 53:1:1872:A:H2'  | 53:1:1873:G:O4'  | 2.05                     | 0.57              |
| 1:b:73:ILE:HG12  | 53:1:1490:A:C6   | 2.40                     | 0.56              |
| 42:R:2:ARG:NH2   | 42:R:5:GLY:O     | 2.38                     | 0.56              |
| 53:1:118:A:H2'   | 53:1:120:U:O4    | 2.05                     | 0.56              |
| 53:1:704:G:H1'   | 53:1:727:A:N6    | 2.19                     | 0.56              |
| 57:7:51:U:H2'    | 57:7:52:G:H8     | 1.70                     | 0.56              |
| 4:e:45:ASP:HB3   | 4:e:48:LEU:HB2   | 1.87                     | 0.56              |
| 19:t:68:LYS:HG3  | 19:t:69:ARG:H    | 1.70                     | 0.56              |
| 20:u:2:ALA:HB3   | 20:u:5:ARG:HE    | 1.68                     | 0.56              |
| 28:D:34:ARG:HH11 | 28:D:39:ARG:NE   | 2.03                     | 0.56              |
| 53:1:2070:A:H2'  | 53:1:2071:A:O4'  | 2.05                     | 0.56              |
| 53:1:2180:U:H2'  | 53:1:2181:U:O4'  | 2.05                     | 0.56              |
| 26:B:8:THR:HG22  | 53:1:2020:A:H5'  | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:G:24:PRO:HB3   | 52:3:828:U:H2'    | 1.86                     | 0.56              |
| 37:M:44:PHE:HB3   | 37:M:45:ILE:HD12  | 1.86                     | 0.56              |
| 39:O:52:LEU:HB2   | 43:S:80:ARG:HD2   | 1.87                     | 0.56              |
| 42:R:3:ILE:HG13   | 42:R:56:ARG:HG2   | 1.87                     | 0.56              |
| 48:X:18:VAL:HG21  | 48:X:43:MET:HE3   | 1.87                     | 0.56              |
| 52:3:1340:A:O2'   | 52:3:1341:U:H5'   | 2.05                     | 0.56              |
| 52:3:1346:A:H2'   | 52:3:1346:A:N3    | 2.21                     | 0.56              |
| 52:3:1346:A:C2'   | 52:3:1347:G:H4'   | 2.33                     | 0.56              |
| 53:1:1045:C:OP1   | 53:1:1047:G:H5'   | 2.05                     | 0.56              |
| 53:1:2834:G:O2'   | 53:1:2835:A:H5'   | 2.05                     | 0.56              |
| 54:2:48:U:H2'     | 54:2:49:C:C6      | 2.40                     | 0.56              |
| 2:c:121:THR:HB    | 2:c:127:PHE:CD2   | 2.40                     | 0.56              |
| 7:h:56:ARG:HG2    | 53:1:1084:A:O4'   | 2.04                     | 0.56              |
| 44:T:68:TYR:HB2   | 52:3:754:C:H4'    | 1.88                     | 0.56              |
| 53:1:1509:A:H2'   | 53:1:1510:G:C8    | 2.40                     | 0.56              |
| 53:1:2112:G:H2'   | 53:1:2113:U:H5'   | 1.86                     | 0.56              |
| 41:Q:112:ALA:HB2  | 52:3:503:C:OP2    | 2.06                     | 0.56              |
| 52:3:335:C:H2'    | 52:3:336:A:C8     | 2.40                     | 0.56              |
| 52:3:1354:U:H2'   | 52:3:1355:G:C8    | 2.40                     | 0.56              |
| 53:1:796:C:H2'    | 53:1:797:G:C8     | 2.41                     | 0.56              |
| 9:j:2:LYS:HA      | 53:1:995:C:H42    | 1.70                     | 0.56              |
| 9:j:27:ARG:HH22   | 53:1:1142:A:H4'   | 1.70                     | 0.56              |
| 44:T:7:THR:HG22   | 44:T:30:LEU:HD11  | 1.87                     | 0.56              |
| 44:T:44:GLU:HG2   | 44:T:45:HIS:N     | 2.21                     | 0.56              |
| 31:G:182:VAL:HG23 | 31:G:195:VAL:HG13 | 1.86                     | 0.56              |
| 41:Q:53:ARG:HG2   | 41:Q:61:GLU:OE2   | 2.05                     | 0.56              |
| 52:3:521:G:O2'    | 52:3:522:C:H5'    | 2.06                     | 0.56              |
| 53:1:2055:C:H2'   | 53:1:2504:U:H5'   | 1.88                     | 0.56              |
| 53:1:2555:U:H2'   | 53:1:2556:C:H5'   | 1.88                     | 0.56              |
| 10:k:12:ASP:HB2   | 10:k:96:GLY:HA3   | 1.87                     | 0.56              |
| 46:V:30:HIS:HD2   | 46:V:33:TYR:H     | 1.54                     | 0.56              |
| 52:3:151:A:H62    | 52:3:170:U:H3     | 1.53                     | 0.56              |
| 53:1:27:G:N2      | 53:1:512:G:H1'    | 2.21                     | 0.56              |
| 20:u:13:LEU:HD11  | 20:u:70:ALA:HB2   | 1.87                     | 0.56              |
| 32:H:175:HIS:NE2  | 52:3:1190:G:H5''  | 2.20                     | 0.56              |
| 49:Y:31:ILE:HD13  | 49:Y:74:HIS:CE1   | 2.40                     | 0.56              |
| 49:Y:48:LYS:HA    | 49:Y:51:ASN:HD21  | 1.70                     | 0.56              |
| 52:3:634:C:H2'    | 52:3:635:A:C8     | 2.41                     | 0.56              |
| 57:7:25:C:C3'     | 57:7:26:A:H5''    | 2.32                     | 0.56              |
| 3:d:149:ILE:HG23  | 3:d:188:MET:HA    | 1.88                     | 0.56              |
| 52:3:381:C:H2'    | 52:3:382:A:O4'    | 2.06                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:3:513:C:H2'    | 52:3:514:C:C6     | 2.41                     | 0.56              |
| 7:h:55:VAL:HA     | 53:1:1084:A:H4'   | 1.87                     | 0.55              |
| 28:D:26:ASN:CG    | 53:1:682:G:H5'    | 2.31                     | 0.55              |
| 31:G:100:LEU:HD22 | 31:G:157:PRO:HG3  | 1.88                     | 0.55              |
| 52:3:1088:G:H21   | 52:3:1167:A:H61   | 1.54                     | 0.55              |
| 53:1:1111:A:H2'   | 53:1:1111:A:N3    | 2.20                     | 0.55              |
| 54:2:108:A:H5'    | 54:2:109:A:O5'    | 2.07                     | 0.55              |
| 55:6:59:A:H2'     | 55:6:60:U:H5'     | 1.88                     | 0.55              |
| 2:c:59:ARG:HH11   | 53:1:2830:C:H3'   | 1.70                     | 0.55              |
| 5:f:41:GLU:HB2    | 5:f:54:ARG:HE     | 1.72                     | 0.55              |
| 34:J:44:ARG:HH21  | 34:J:70:MET:HG3   | 1.71                     | 0.55              |
| 34:J:108:GLY:H    | 52:3:9:G:H4'      | 1.70                     | 0.55              |
| 21:v:4:ILE:HG21   | 21:v:42:LEU:HD22  | 1.89                     | 0.55              |
| 33:I:40:HIS:HD2   | 33:I:43:ARG:HE    | 1.54                     | 0.55              |
| 38:N:59:LYS:C     | 38:N:60:LEU:HD22  | 2.31                     | 0.55              |
| 52:3:32:A:H2'     | 52:3:33:A:C8      | 2.41                     | 0.55              |
| 52:3:1105:A:H2'   | 52:3:1106:G:C8    | 2.41                     | 0.55              |
| 53:1:532:A:H2'    | 53:1:532:A:N3     | 2.21                     | 0.55              |
| 30:F:16:ILE:N     | 30:F:16:ILE:HD12  | 2.20                     | 0.55              |
| 52:3:216:U:H2'    | 52:3:217:C:C6     | 2.41                     | 0.55              |
| 53:1:323:C:H2'    | 53:1:1205:A:H61   | 1.71                     | 0.55              |
| 53:1:828:U:H4'    | 53:1:831:G:C2     | 2.42                     | 0.55              |
| 53:1:834:G:H1'    | 53:1:2358:A:N3    | 2.21                     | 0.55              |
| 32:H:155:ARG:O    | 32:H:156:LEU:HD23 | 2.06                     | 0.55              |
| 33:I:30:LYS:HD2   | 52:3:413:G:N7     | 2.22                     | 0.55              |
| 38:N:11:ARG:HA    | 38:N:105:ARG:HH12 | 1.72                     | 0.55              |
| 41:Q:33:CYS:HA    | 41:Q:54:VAL:HA    | 1.89                     | 0.55              |
| 42:R:93:GLY:O     | 42:R:108:ARG:HG3  | 2.07                     | 0.55              |
| 52:3:112:G:H21    | 52:3:354:G:H5'    | 1.71                     | 0.55              |
| 53:1:2146:C:H4'   | 53:1:2147:A:C5    | 2.41                     | 0.55              |
| 55:6:71:C:H2'     | 55:6:72:A:C8      | 2.42                     | 0.55              |
| 2:c:123:LYS:HG2   | 2:c:165:MET:HE1   | 1.88                     | 0.55              |
| 6:g:97:ARG:HH21   | 53:1:2220:U:H5'   | 1.71                     | 0.55              |
| 9:j:113:PRO:HD2   | 53:1:558:U:P      | 2.47                     | 0.55              |
| 21:v:6:ALA:HB2    | 21:v:42:LEU:HB3   | 1.88                     | 0.55              |
| 38:N:56:MET:HG3   | 38:N:57:VAL:N     | 2.22                     | 0.55              |
| 40:P:126:ARG:NH2  | 52:3:692:U:H5''   | 2.22                     | 0.55              |
| 52:3:1060:U:H2'   | 52:3:1061:G:H8    | 1.72                     | 0.55              |
| 53:1:18:U:H2'     | 53:1:19:A:C8      | 2.41                     | 0.55              |
| 53:1:215:G:C4'    | 53:1:216:A:H4'    | 2.36                     | 0.55              |
| 53:1:635:C:H2'    | 53:1:636:G:C8     | 2.41                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:720:U:H2'    | 53:1:721:A:C8     | 2.42                     | 0.55              |
| 2:c:20:VAL:HG23   | 10:k:72:PRO:HB2   | 1.89                     | 0.55              |
| 9:j:26:GLY:HA3    | 53:1:1140:C:C5'   | 2.37                     | 0.55              |
| 39:O:48:ARG:HH11  | 39:O:48:ARG:HG3   | 1.72                     | 0.55              |
| 52:3:950:U:H2'    | 52:3:951:G:C8     | 2.42                     | 0.55              |
| 54:2:30:C:H2'     | 54:2:31:C:O4'     | 2.06                     | 0.55              |
| 58:8:113:MET:HB2  | 58:8:116:THR:HG23 | 1.88                     | 0.55              |
| 23:x:9:LYS:HG2    | 53:1:396:G:OP1    | 2.07                     | 0.55              |
| 32:H:109:GLU:HB2  | 32:H:143:LEU:HD22 | 1.88                     | 0.55              |
| 49:Y:43:LYS:HG3   | 49:Y:86:ALA:HB3   | 1.89                     | 0.55              |
| 52:3:337:G:H2'    | 52:3:338:A:C8     | 2.41                     | 0.55              |
| 23:x:16:ASN:HB3   | 23:x:24:THR:HG23  | 1.89                     | 0.55              |
| 32:H:102:ILE:HD12 | 32:H:102:ILE:N    | 2.22                     | 0.55              |
| 34:J:23:THR:HA    | 34:J:28:ARG:HA    | 1.88                     | 0.55              |
| 49:Y:25:SER:OG    | 52:3:1458:G:H5''  | 2.07                     | 0.55              |
| 53:1:2743:U:H2'   | 53:1:2744:G:H5''  | 1.88                     | 0.55              |
| 54:2:2:G:H2'      | 54:2:3:C:C6       | 2.42                     | 0.55              |
| 1:b:47:ARG:HD3    | 53:1:778:G:H5''   | 1.88                     | 0.55              |
| 9:j:11:VAL:HG21   | 9:j:50:THR:HA     | 1.88                     | 0.55              |
| 11:l:111:ILE:HD11 | 53:1:636:G:C6     | 2.43                     | 0.55              |
| 52:3:12:U:H4'     | 52:3:526:C:H4'    | 1.89                     | 0.55              |
| 52:3:358:U:H2'    | 52:3:359:G:C8     | 2.41                     | 0.55              |
| 52:3:410:G:H2'    | 52:3:429:U:O4     | 2.07                     | 0.55              |
| 53:1:381:G:H2'    | 53:1:382:A:H8     | 1.72                     | 0.55              |
| 53:1:1856:U:H2'   | 53:1:1857:G:O4'   | 2.07                     | 0.55              |
| 53:1:2266:A:H4'   | 53:1:2267:A:N3    | 2.22                     | 0.55              |
| 54:2:4:C:H2'      | 54:2:5:U:C6       | 2.41                     | 0.55              |
| 29:E:32:LEU:HB3   | 29:E:40:LYS:HD3   | 1.89                     | 0.54              |
| 31:G:116:LEU:HB3  | 31:G:140:LEU:HD13 | 1.89                     | 0.54              |
| 45:U:75:ILE:O     | 45:U:78:VAL:HG12  | 2.07                     | 0.54              |
| 52:3:1391:U:H2'   | 52:3:1392:G:C8    | 2.42                     | 0.54              |
| 52:3:1497:G:C2'   | 52:3:1498:U:H5'   | 2.37                     | 0.54              |
| 53:1:2329:U:H2'   | 53:1:2330:G:C8    | 2.42                     | 0.54              |
| 53:1:2345:G:N3    | 53:1:2381:A:H2'   | 2.22                     | 0.54              |
| 1:b:68:ARG:O      | 1:b:188:ARG:NH1   | 2.41                     | 0.54              |
| 30:F:17:VAL:CG1   | 30:F:19:ARG:HG3   | 2.36                     | 0.54              |
| 45:U:26:ASN:HD22  | 45:U:31:ARG:HB3   | 1.72                     | 0.54              |
| 46:V:26:ARG:NH2   | 52:3:237:G:H5''   | 2.23                     | 0.54              |
| 52:3:418:C:H2'    | 52:3:419:C:C6     | 2.43                     | 0.54              |
| 52:3:695:A:H2'    | 52:3:696:A:C8     | 2.42                     | 0.54              |
| 53:1:2671:G:H2'   | 53:1:2672:U:C6    | 2.42                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 12:m:53:MET:HE1   | 12:m:103:TYR:HB3 | 1.89                     | 0.54              |
| 52:3:1306:A:N6    | 52:3:1331:G:H1'  | 2.22                     | 0.54              |
| 53:1:323:C:H2'    | 53:1:1205:A:N6   | 2.22                     | 0.54              |
| 37:M:40:LYS:HZ3   | 37:M:48:PHE:HE1  | 1.55                     | 0.54              |
| 40:P:30:ILE:HG23  | 40:P:45:THR:HG22 | 1.89                     | 0.54              |
| 52:3:79:G:O2'     | 52:3:80:A:H5'    | 2.08                     | 0.54              |
| 2:c:124:ARG:HA    | 2:c:165:MET:SD   | 2.47                     | 0.54              |
| 33:I:82:LYS:HZ2   | 52:3:5:U:H5      | 1.55                     | 0.54              |
| 35:K:64:VAL:HG22  | 35:K:65:GLU:H    | 1.73                     | 0.54              |
| 52:3:59:A:H3'     | 52:3:331:G:H22   | 1.72                     | 0.54              |
| 52:3:411:A:C4     | 52:3:413:G:H1'   | 2.43                     | 0.54              |
| 52:3:673:A:H2'    | 52:3:674:G:C8    | 2.42                     | 0.54              |
| 53:1:1668:A:H61   | 53:1:1676:A:H61  | 1.55                     | 0.54              |
| 53:1:1971:U:H5'   | 53:1:1972:G:H5'' | 1.88                     | 0.54              |
| 7:h:23:LEU:HD12   | 7:h:117:LEU:O    | 2.08                     | 0.54              |
| 10:k:34:GLY:H     | 10:k:37:ASP:CG   | 2.16                     | 0.54              |
| 10:k:98:ARG:HH21  | 52:3:339:C:P     | 2.31                     | 0.54              |
| 14:o:9:ARG:NH2    | 53:1:2296:U:O4   | 2.39                     | 0.54              |
| 15:p:25:VAL:HG22  | 15:p:26:GLU:N    | 2.22                     | 0.54              |
| 16:q:111:LYS:HG2  | 17:r:48:LYS:HE3  | 1.89                     | 0.54              |
| 45:U:46:LYS:HE3   | 52:3:617:G:H5'   | 1.89                     | 0.54              |
| 1:b:42:ARG:NH1    | 53:1:690:G:H21   | 2.05                     | 0.54              |
| 1:b:226:PRO:HD3   | 1:b:233:GLY:HA2  | 1.89                     | 0.54              |
| 5:f:175:LYS:HZ1   | 53:1:2473:U:H3   | 1.54                     | 0.54              |
| 9:j:15:TRP:HB3    | 9:j:137:PRO:HB3  | 1.90                     | 0.54              |
| 31:G:119:GLN:HE22 | 31:G:136:ARG:NH1 | 2.05                     | 0.54              |
| 42:R:105:ALA:HA   | 52:3:948:C:OP1   | 2.07                     | 0.54              |
| 53:1:2281:A:O2'   | 53:1:2282:G:H5'  | 2.07                     | 0.54              |
| 6:g:8:LYS:O       | 6:g:9:VAL:C      | 2.49                     | 0.54              |
| 35:K:18:VAL:HG11  | 35:K:58:HIS:CD2  | 2.42                     | 0.54              |
| 36:L:24:LYS:HA    | 36:L:27:ASN:HD22 | 1.73                     | 0.54              |
| 53:1:1563:U:H2'   | 53:1:1564:C:C6   | 2.43                     | 0.54              |
| 7:h:118:ILE:HG22  | 7:h:119:PRO:CD   | 2.38                     | 0.54              |
| 28:D:34:ARG:HH22  | 53:1:466:A:P     | 2.31                     | 0.54              |
| 35:K:64:VAL:HG22  | 35:K:65:GLU:N    | 2.22                     | 0.54              |
| 48:X:24:SER:CB    | 48:X:27:LYS:HE3  | 2.36                     | 0.54              |
| 52:3:621:A:H2'    | 52:3:622:A:C8    | 2.43                     | 0.54              |
| 5:f:32:LEU:HD23   | 5:f:74:MET:HG2   | 1.89                     | 0.54              |
| 13:n:31:HIS:O     | 13:n:32:GLU:HB2  | 2.08                     | 0.54              |
| 30:F:36:ARG:HD2   | 30:F:36:ARG:C    | 2.33                     | 0.54              |
| 38:N:121:ARG:NH1  | 52:3:1345:U:H5'' | 2.23                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 52:3:1015:G:O2'  | 52:3:1016:A:H5'  | 2.07                     | 0.54              |
| 52:3:1273:C:H2'  | 52:3:1274:A:O4'  | 2.08                     | 0.54              |
| 53:1:821:A:H5''  | 53:1:822:G:H5'   | 1.89                     | 0.54              |
| 53:1:828:U:H4'   | 53:1:831:G:N1    | 2.23                     | 0.54              |
| 53:1:1827:U:H2'  | 53:1:1828:G:O4'  | 2.07                     | 0.54              |
| 53:1:2339:C:H2'  | 53:1:2340:A:H8   | 1.73                     | 0.54              |
| 55:5:76:A:H5'    | 55:5:76:A:C8     | 2.43                     | 0.54              |
| 4:e:107:VAL:HG22 | 4:e:108:PRO:HD3  | 1.89                     | 0.53              |
| 15:p:54:LEU:HD23 | 15:p:54:LEU:O    | 2.07                     | 0.53              |
| 19:t:11:LEU:HD11 | 19:t:32:LEU:HD22 | 1.90                     | 0.53              |
| 19:t:56:GLU:HB3  | 19:t:86:THR:HG23 | 1.89                     | 0.53              |
| 38:N:114:LYS:NZ  | 52:3:1186:G:O2'  | 2.41                     | 0.53              |
| 52:3:1427:C:H2'  | 52:3:1428:A:C8   | 2.43                     | 0.53              |
| 53:1:278:A:H2'   | 53:1:278:A:N3    | 2.23                     | 0.53              |
| 53:1:669:G:H2'   | 53:1:669:G:N3    | 2.23                     | 0.53              |
| 53:1:898:C:H2'   | 53:1:899:A:O4'   | 2.08                     | 0.53              |
| 53:1:2537:U:H2'  | 53:1:2538:C:C6   | 2.43                     | 0.53              |
| 53:1:2743:U:C3'  | 53:1:2744:G:H5'' | 2.38                     | 0.53              |
| 1:b:83:ASP:OD1   | 1:b:86:ARG:HD3   | 2.07                     | 0.53              |
| 7:h:56:ARG:CZ    | 7:h:83:ALA:HB2   | 2.38                     | 0.53              |
| 10:k:32:TYR:HH   | 53:1:1996:C:H5   | 1.56                     | 0.53              |
| 31:G:166:ASP:HB2 | 31:G:190:SER:HA  | 1.90                     | 0.53              |
| 33:I:57:LYS:O    | 33:I:60:VAL:HG12 | 2.08                     | 0.53              |
| 41:Q:113:ARG:HB2 | 41:Q:118:VAL:HB  | 1.90                     | 0.53              |
| 52:3:876:C:H2'   | 52:3:877:G:C8    | 2.43                     | 0.53              |
| 53:1:1105:U:H2'  | 53:1:1106:G:H5'' | 1.90                     | 0.53              |
| 53:1:1386:C:H2'  | 53:1:1387:A:H8   | 1.72                     | 0.53              |
| 1:b:256:THR:OG1  | 53:1:1798:U:H5'  | 2.09                     | 0.53              |
| 3:d:69:ARG:HD3   | 53:1:674:G:H1'   | 1.90                     | 0.53              |
| 4:e:34:THR:HB    | 4:e:154:THR:HB   | 1.89                     | 0.53              |
| 26:B:49:ARG:HG2  | 53:1:2884:U:C6   | 2.43                     | 0.53              |
| 53:1:1300:G:C4'  | 53:1:1301:A:H5'' | 2.38                     | 0.53              |
| 53:1:2128:G:H1'  | 53:1:2173:A:N3   | 2.22                     | 0.53              |
| 53:1:2328:A:H2'  | 53:1:2329:U:C6   | 2.42                     | 0.53              |
| 53:1:2389:G:H5'' | 53:1:2390:U:O4'  | 2.08                     | 0.53              |
| 53:1:2623:G:H2'  | 53:1:2624:G:H8   | 1.74                     | 0.53              |
| 58:8:313:SER:HA  | 58:8:353:PRO:HB3 | 1.89                     | 0.53              |
| 3:d:1:MET:N      | 3:d:14:VAL:O     | 2.41                     | 0.53              |
| 20:u:4:ILE:HD12  | 20:u:4:ILE:N     | 2.24                     | 0.53              |
| 39:O:72:ARG:NH2  | 52:3:1151:A:O2'  | 2.41                     | 0.53              |
| 44:T:44:GLU:HG2  | 44:T:45:HIS:CD2  | 2.44                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:3:1391:U:H2'   | 52:3:1392:G:H8    | 1.72                     | 0.53              |
| 53:1:304:U:H2'    | 53:1:305:C:C6     | 2.44                     | 0.53              |
| 33:I:37:PRO:HD2   | 33:I:41:GLY:CA    | 2.39                     | 0.53              |
| 41:Q:54:VAL:HG22  | 41:Q:55:ARG:N     | 2.23                     | 0.53              |
| 50:Z:48:LYS:HE2   | 52:3:724:G:OP1    | 2.08                     | 0.53              |
| 52:3:225:C:H2'    | 52:3:226:G:C5'    | 2.38                     | 0.53              |
| 52:3:1139:G:H5''  | 52:3:1140:C:H5    | 1.72                     | 0.53              |
| 52:3:1200:C:H5''  | 52:3:1201:A:H3'   | 1.91                     | 0.53              |
| 53:1:367:G:H2'    | 53:1:368:A:O4'    | 2.08                     | 0.53              |
| 53:1:1420:A:H5'   | 53:1:1421:G:OP2   | 2.09                     | 0.53              |
| 53:1:1772:A:H2'   | 53:1:1773:A:H4'   | 1.90                     | 0.53              |
| 53:1:1844:C:H2'   | 53:1:1845:G:H8    | 1.72                     | 0.53              |
| 53:1:2233:U:H2'   | 53:1:2234:G:H8    | 1.74                     | 0.53              |
| 37:M:82:LEU:HD13  | 41:Q:3:VAL:HG21   | 1.90                     | 0.53              |
| 43:S:20:PHE:O     | 43:S:21:ALA:HB3   | 2.09                     | 0.53              |
| 52:3:5:U:H4'      | 52:3:6:G:C4       | 2.44                     | 0.53              |
| 52:3:235:C:H2'    | 52:3:236:A:H8     | 1.74                     | 0.53              |
| 2:c:135:GLY:HA2   | 53:1:743:A:OP1    | 2.08                     | 0.53              |
| 7:h:23:LEU:HD13   | 7:h:118:ILE:CG1   | 2.38                     | 0.53              |
| 11:l:95:LEU:HD22  | 11:l:100:ILE:HD11 | 1.90                     | 0.53              |
| 13:n:24:MET:HE3   | 13:n:44:LEU:HD13  | 1.89                     | 0.53              |
| 15:p:50:ARG:NH1   | 53:1:2684:U:OP2   | 2.42                     | 0.53              |
| 15:p:102:ARG:HH11 | 15:p:106:ALA:HB1  | 1.71                     | 0.53              |
| 39:O:59:LYS:O     | 39:O:62:ARG:NH1   | 2.42                     | 0.53              |
| 42:R:97:ARG:HB2   | 42:R:99:GLN:NE2   | 2.17                     | 0.53              |
| 44:T:54:GLY:O     | 44:T:58:MET:HG3   | 2.08                     | 0.53              |
| 51:a:193:LEU:O    | 51:a:196:LEU:HG   | 2.09                     | 0.53              |
| 52:3:367:U:H5'    | 58:8:280:ARG:HH21 | 1.74                     | 0.53              |
| 53:1:546:U:H2'    | 53:1:547:A:C4'    | 2.39                     | 0.53              |
| 53:1:742:A:H2'    | 53:1:743:A:C8     | 2.44                     | 0.53              |
| 53:1:1524:G:H2'   | 53:1:1525:A:C8    | 2.43                     | 0.53              |
| 53:1:2257:U:O2'   | 53:1:2258:C:H5'   | 2.08                     | 0.53              |
| 53:1:2391:G:H1'   | 53:1:2429:G:N2    | 2.24                     | 0.53              |
| 6:g:31:VAL:CG1    | 6:g:32:PRO:HD3    | 2.39                     | 0.53              |
| 42:R:95:PRO:HG2   | 42:R:105:ALA:HB1  | 1.91                     | 0.53              |
| 45:U:21:VAL:HG23  | 45:U:33:ILE:HB    | 1.90                     | 0.53              |
| 53:1:1367:A:C2'   | 53:1:1368:G:H5'   | 2.38                     | 0.53              |
| 9:j:44:TYR:O      | 16:q:63:ARG:NE    | 2.39                     | 0.53              |
| 10:k:10:VAL:HG11  | 10:k:16:ALA:HB3   | 1.91                     | 0.53              |
| 15:p:49:ILE:HG22  | 15:p:58:PHE:HB2   | 1.91                     | 0.53              |
| 32:H:18:ASN:ND2   | 43:S:89:ARG:O     | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 52:3:70:U:H5''   | 52:3:71:A:OP1    | 2.09                     | 0.53              |
| 52:3:1106:G:O2'  | 52:3:1107:C:H5'  | 2.09                     | 0.53              |
| 52:3:1513:A:H2'  | 52:3:1514:G:H8   | 1.73                     | 0.53              |
| 53:1:1720:U:H2'  | 53:1:1721:G:O4'  | 2.09                     | 0.53              |
| 53:1:2801:G:H2'  | 53:1:2802:G:C8   | 2.44                     | 0.53              |
| 1:b:216:ARG:NH2  | 53:1:781:A:OP1   | 2.42                     | 0.53              |
| 35:K:75:GLU:HA   | 35:K:78:PHE:HD2  | 1.74                     | 0.53              |
| 42:R:85:TYR:H    | 48:X:72:GLU:HB3  | 1.74                     | 0.53              |
| 52:3:390:U:H2'   | 52:3:391:G:H8    | 1.72                     | 0.53              |
| 58:8:378:ARG:NH1 | 58:8:383:THR:OG1 | 2.42                     | 0.53              |
| 6:g:73:ASN:HD22  | 6:g:76:GLU:HA    | 1.74                     | 0.52              |
| 26:B:42:ILE:HG22 | 26:B:48:TYR:HB2  | 1.91                     | 0.52              |
| 30:F:16:ILE:HD12 | 30:F:16:ILE:H    | 1.74                     | 0.52              |
| 33:I:59:LYS:O    | 33:I:63:ILE:HG12 | 2.09                     | 0.52              |
| 38:N:64:ILE:HD12 | 38:N:64:ILE:N    | 2.23                     | 0.52              |
| 40:P:19:VAL:HG12 | 40:P:82:GLU:HB2  | 1.90                     | 0.52              |
| 52:3:390:U:H2'   | 52:3:391:G:C8    | 2.44                     | 0.52              |
| 52:3:1540:U:O2   | 52:3:1540:U:H3'  | 2.09                     | 0.52              |
| 53:1:745:G:O2'   | 53:1:748:G:H1'   | 2.08                     | 0.52              |
| 53:1:2208:C:H2'  | 53:1:2209:G:H8   | 1.74                     | 0.52              |
| 4:e:48:LEU:HA    | 4:e:51:ASN:HD22  | 1.74                     | 0.52              |
| 16:q:23:TYR:CD1  | 53:1:533:G:H5'   | 2.44                     | 0.52              |
| 33:I:58:GLN:O    | 33:I:62:ARG:HG2  | 2.10                     | 0.52              |
| 35:K:2:ARG:HG3   | 35:K:68:GLN:HE21 | 1.73                     | 0.52              |
| 53:1:441:U:O2'   | 53:1:442:G:H5'   | 2.09                     | 0.52              |
| 53:1:511:U:H2'   | 53:1:512:G:H5'   | 1.91                     | 0.52              |
| 53:1:1657:U:H2'  | 53:1:1658:C:C6   | 2.44                     | 0.52              |
| 53:1:2073:C:O2'  | 53:1:2074:U:H5'  | 2.09                     | 0.52              |
| 55:6:37:A:O2'    | 55:6:38:A:H5'    | 2.09                     | 0.52              |
| 58:8:187:ALA:O   | 58:8:191:GLU:HG3 | 2.09                     | 0.52              |
| 6:g:5:LEU:HD22   | 6:g:13:GLY:HA2   | 1.91                     | 0.52              |
| 14:o:16:ARG:O    | 14:o:20:GLU:HG2  | 2.09                     | 0.52              |
| 16:q:91:ARG:HH12 | 53:1:997:G:H5''  | 1.74                     | 0.52              |
| 30:F:7:VAL:HB    | 30:F:35:GLN:NE2  | 2.24                     | 0.52              |
| 35:K:73:GLU:O    | 35:K:76:THR:OG1  | 2.28                     | 0.52              |
| 39:O:71:LEU:O    | 39:O:72:ARG:NH1  | 2.41                     | 0.52              |
| 40:P:92:ARG:HH22 | 50:Z:24:LYS:HG3  | 1.74                     | 0.52              |
| 45:U:5:ARG:NH1   | 52:3:377:G:H5'   | 2.25                     | 0.52              |
| 45:U:17:TYR:HB2  | 45:U:39:PHE:HB3  | 1.90                     | 0.52              |
| 52:3:422:C:H5''  | 52:3:423:G:O5'   | 2.10                     | 0.52              |
| 52:3:539:A:H2'   | 52:3:540:G:C8    | 2.45                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 52:3:1171:A:H2'   | 52:3:1172:C:C6   | 2.44                     | 0.52              |
| 53:1:226:A:H2'    | 53:1:227:A:O4'   | 2.09                     | 0.52              |
| 53:1:467:G:O2'    | 53:1:468:G:H5'   | 2.09                     | 0.52              |
| 53:1:2248:C:C2'   | 53:1:2249:U:H5'  | 2.38                     | 0.52              |
| 58:8:164:PRO:HB2  | 58:8:167:ASP:HB3 | 1.91                     | 0.52              |
| 3:d:176:ASP:N     | 3:d:176:ASP:OD1  | 2.42                     | 0.52              |
| 16:q:50:ARG:HH11  | 16:q:50:ARG:HG3  | 1.74                     | 0.52              |
| 53:1:458:G:O2'    | 53:1:459:U:H5    | 1.93                     | 0.52              |
| 53:1:720:U:H2'    | 53:1:721:A:H8    | 1.73                     | 0.52              |
| 7:h:67:THR:HG22   | 7:h:72:LEU:HA    | 1.92                     | 0.52              |
| 8:i:91:LYS:HB3    | 8:i:94:LYS:HB2   | 1.92                     | 0.52              |
| 11:l:101:ILE:HG13 | 11:l:102:GLY:N   | 2.24                     | 0.52              |
| 45:U:52:LEU:HD12  | 45:U:57:ILE:HD11 | 1.91                     | 0.52              |
| 51:a:53:ARG:HB3   | 55:6:62:C:H4'    | 1.90                     | 0.52              |
| 52:3:279:A:H5'    | 52:3:281:G:C5'   | 2.38                     | 0.52              |
| 53:1:1434:A:H2'   | 53:1:1435:G:C8   | 2.45                     | 0.52              |
| 53:1:2183:A:H2'   | 53:1:2184:A:C8   | 2.45                     | 0.52              |
| 53:1:2208:C:H2'   | 53:1:2209:G:C8   | 2.44                     | 0.52              |
| 53:1:2660:A:N1    | 57:7:62:C:H4'    | 2.25                     | 0.52              |
| 54:2:104:A:H2'    | 54:2:105:G:O4'   | 2.09                     | 0.52              |
| 32:H:30:ASP:HA    | 43:S:64:ARG:HH12 | 1.74                     | 0.52              |
| 33:I:89:LEU:O     | 33:I:93:LEU:HD23 | 2.10                     | 0.52              |
| 44:T:64:LYS:O     | 44:T:67:ASP:OD1  | 2.27                     | 0.52              |
| 52:3:224:U:H2'    | 52:3:225:C:C6    | 2.44                     | 0.52              |
| 53:1:2241:A:H2'   | 53:1:2242:G:C8   | 2.44                     | 0.52              |
| 53:1:2371:G:O2'   | 53:1:2372:U:H5'  | 2.09                     | 0.52              |
| 13:n:1:MET:H2     | 53:1:1654:A:P    | 2.31                     | 0.52              |
| 30:F:9:LYS:HD3    | 30:F:16:ILE:HD11 | 1.91                     | 0.52              |
| 31:G:132:GLU:HA   | 31:G:135:MET:HE3 | 1.92                     | 0.52              |
| 33:I:143:SER:HB2  | 33:I:178:GLU:OE1 | 2.10                     | 0.52              |
| 36:L:68:VAL:HG23  | 36:L:99:ALA:HB1  | 1.91                     | 0.52              |
| 40:P:58:THR:HG23  | 40:P:61:ALA:H    | 1.75                     | 0.52              |
| 52:3:181:A:H61    | 52:3:194:C:H2'   | 1.73                     | 0.52              |
| 52:3:1527:U:O2'   | 52:3:1528:U:H5'  | 2.09                     | 0.52              |
| 53:1:1097:U:H2'   | 53:1:1098:A:O4'  | 2.09                     | 0.52              |
| 58:8:154:VAL:O    | 58:8:157:LEU:HG  | 2.10                     | 0.52              |
| 30:F:7:VAL:HG11   | 30:F:35:GLN:HB2  | 1.92                     | 0.52              |
| 39:O:66:GLU:HG2   | 43:S:98:ALA:HB2  | 1.92                     | 0.52              |
| 53:1:784:G:HO2'   | 53:1:785:G:H8    | 1.58                     | 0.52              |
| 53:1:1138:G:H2'   | 53:1:1139:G:O4'  | 2.09                     | 0.52              |
| 53:1:2011:U:H2'   | 53:1:2012:G:O4'  | 2.10                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:E:63:TYR:OH   | 53:1:593:U:H5'    | 2.10                     | 0.52              |
| 33:I:173:ASP:OD2 | 33:I:176:LYS:HG2  | 2.09                     | 0.52              |
| 41:Q:41:PRO:HG3  | 41:Q:49:ARG:HG3   | 1.91                     | 0.52              |
| 52:3:368:U:OP2   | 58:8:257:THR:HG21 | 2.09                     | 0.52              |
| 53:1:687:C:H2'   | 53:1:688:U:O4'    | 2.10                     | 0.52              |
| 53:1:1857:G:H1'  | 53:1:1885:A:N6    | 2.25                     | 0.52              |
| 4:e:154:THR:HG21 | 53:1:2314:A:O4'   | 2.10                     | 0.52              |
| 12:m:11:LYS:HE3  | 12:m:86:LYS:HB3   | 1.92                     | 0.52              |
| 14:o:6:ALA:HA    | 14:o:9:ARG:HG2    | 1.90                     | 0.52              |
| 18:s:36:LEU:HA   | 18:s:39:THR:HG22  | 1.91                     | 0.52              |
| 28:D:11:LYS:CE   | 53:1:686:U:H5''   | 2.38                     | 0.52              |
| 32:H:40:GLN:O    | 32:H:44:LYS:HG2   | 2.10                     | 0.52              |
| 33:I:37:PRO:HD2  | 33:I:41:GLY:HA2   | 1.90                     | 0.52              |
| 38:N:57:VAL:HG22 | 38:N:59:LYS:HZ3   | 1.75                     | 0.52              |
| 39:O:37:ARG:HG3  | 52:3:1124:G:H5''  | 1.91                     | 0.52              |
| 41:Q:51:VAL:HG22 | 41:Q:52:CYS:N     | 2.25                     | 0.52              |
| 41:Q:85:ARG:HH21 | 41:Q:87:LYS:HB2   | 1.75                     | 0.52              |
| 53:1:2655:G:HO2' | 53:1:2656:U:H5    | 1.58                     | 0.52              |
| 1:b:158:GLY:H    | 1:b:194:VAL:HG23  | 1.75                     | 0.51              |
| 5:f:175:LYS:NZ   | 53:1:2473:U:H3    | 2.08                     | 0.51              |
| 7:h:118:ILE:CG2  | 7:h:119:PRO:HD3   | 2.40                     | 0.51              |
| 16:q:23:TYR:CE1  | 53:1:533:G:H5'    | 2.44                     | 0.51              |
| 22:w:62:LYS:HB2  | 22:w:81:GLU:HG3   | 1.92                     | 0.51              |
| 35:K:92:THR:OG1  | 35:K:93:LYS:N     | 2.38                     | 0.51              |
| 38:N:22:PRO:HA   | 38:N:60:LEU:HD13  | 1.92                     | 0.51              |
| 51:a:42:VAL:HG13 | 51:a:178:VAL:HG12 | 1.92                     | 0.51              |
| 53:1:2469:A:H2'  | 53:1:2470:G:O4'   | 2.11                     | 0.51              |
| 53:1:2853:C:H2'  | 53:1:2854:G:H8    | 1.75                     | 0.51              |
| 6:g:31:VAL:HG12  | 6:g:32:PRO:HD3    | 1.92                     | 0.51              |
| 21:v:60:VAL:HG22 | 21:v:73:LYS:HE3   | 1.92                     | 0.51              |
| 33:I:167:PRO:HB2 | 33:I:170:LEU:HD21 | 1.91                     | 0.51              |
| 36:L:3:ARG:NH2   | 52:3:932:C:C5'    | 2.71                     | 0.51              |
| 45:U:58:ALA:HA   | 45:U:61:VAL:HG22  | 1.92                     | 0.51              |
| 51:a:205:LYS:HB3 | 53:1:1860:G:O3'   | 2.10                     | 0.51              |
| 52:3:128:G:O2'   | 52:3:129:A:H5'    | 2.10                     | 0.51              |
| 52:3:648:A:H2'   | 52:3:649:A:H8     | 1.75                     | 0.51              |
| 53:1:534:U:H2'   | 53:1:535:G:C8     | 2.45                     | 0.51              |
| 53:1:996:A:H2'   | 53:1:997:G:H8     | 1.75                     | 0.51              |
| 53:1:1874:C:H2'  | 53:1:1875:G:O4'   | 2.09                     | 0.51              |
| 53:1:2286:G:H4'  | 53:1:2287:A:O5'   | 2.09                     | 0.51              |
| 58:8:16:GLY:HA2  | 58:8:80:VAL:H     | 1.75                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:b:30:ALA:HB3    | 1:b:31:PRO:HD3   | 1.93                     | 0.51              |
| 4:e:30:VAL:HA     | 4:e:157:THR:HA   | 1.92                     | 0.51              |
| 4:e:90:LEU:HD13   | 4:e:95:MET:HA    | 1.91                     | 0.51              |
| 26:B:54:ILE:HG23  | 26:B:56:LYS:H    | 1.76                     | 0.51              |
| 52:3:570:G:H5'    | 52:3:820:U:O4'   | 2.10                     | 0.51              |
| 55:6:51:C:H2'     | 55:6:52:G:C8     | 2.44                     | 0.51              |
| 8:i:74:PRO:HG3    | 53:1:1060:U:OP1  | 2.11                     | 0.51              |
| 11:l:29:LYS:O     | 11:l:30:THR:OG1  | 2.23                     | 0.51              |
| 19:t:73:ARG:NH1   | 53:1:456:C:C4    | 2.76                     | 0.51              |
| 29:E:57:VAL:HA    | 29:E:60:CYS:SG   | 2.51                     | 0.51              |
| 31:G:5:MET:SD     | 31:G:5:MET:N     | 2.84                     | 0.51              |
| 33:I:149:LYS:O    | 33:I:150:LYS:HG3 | 2.10                     | 0.51              |
| 43:S:84:ARG:HH22  | 52:3:1059:C:H4'  | 1.75                     | 0.51              |
| 52:3:1306:A:H62   | 52:3:1331:G:H1'  | 1.75                     | 0.51              |
| 52:3:1477:U:H2'   | 52:3:1478:U:C6   | 2.45                     | 0.51              |
| 53:1:679:C:H2'    | 53:1:680:C:C6    | 2.46                     | 0.51              |
| 2:c:1:MET:HG3     | 2:c:2:ILE:H      | 1.73                     | 0.51              |
| 4:e:62:GLN:HB3    | 4:e:94:ARG:HH12  | 1.76                     | 0.51              |
| 4:e:107:VAL:HG23  | 4:e:108:PRO:HD3  | 1.92                     | 0.51              |
| 10:k:6:THR:HG23   | 53:1:1666:G:O3'  | 2.10                     | 0.51              |
| 41:Q:113:ARG:HB2  | 41:Q:118:VAL:O   | 2.11                     | 0.51              |
| 53:1:1092:C:H2'   | 53:1:1093:G:O4'  | 2.10                     | 0.51              |
| 53:1:1827:U:O2'   | 53:1:1828:G:H5'  | 2.10                     | 0.51              |
| 53:1:1956:U:H2'   | 53:1:1957:C:H5'  | 1.93                     | 0.51              |
| 1:b:184:GLU:HG3   | 1:b:186:ASP:H    | 1.76                     | 0.51              |
| 2:c:155:VAL:O     | 53:1:2619:C:H5'  | 2.10                     | 0.51              |
| 7:h:117:LEU:HD23  | 7:h:120:ALA:HA   | 1.92                     | 0.51              |
| 7:h:123:ILE:HD12  | 7:h:123:ILE:N    | 2.23                     | 0.51              |
| 9:j:6:ALA:HB3     | 9:j:48:VAL:HG11  | 1.91                     | 0.51              |
| 9:j:78:THR:HB     | 53:1:2641:G:H5'' | 1.92                     | 0.51              |
| 11:l:101:ILE:HG13 | 11:l:102:GLY:H   | 1.76                     | 0.51              |
| 14:o:29:HIS:HB3   | 14:o:36:TYR:HB2  | 1.91                     | 0.51              |
| 22:w:34:VAL:HG22  | 22:w:55:LEU:HB2  | 1.93                     | 0.51              |
| 54:2:3:C:H3'      | 54:2:4:C:C5'     | 2.41                     | 0.51              |
| 21:v:80:HIS:ND1   | 21:v:81:PRO:HD2  | 2.26                     | 0.51              |
| 26:B:47:TYR:CZ    | 26:B:52:LYS:HD3  | 2.45                     | 0.51              |
| 35:K:67:PRO:HB2   | 35:K:69:GLU:OE2  | 2.10                     | 0.51              |
| 41:Q:80:LEU:HB3   | 41:Q:97:VAL:HB   | 1.92                     | 0.51              |
| 44:T:88:ARG:H     | 44:T:88:ARG:HD3  | 1.76                     | 0.51              |
| 45:U:38:PHE:CE1   | 45:U:51:ARG:HB2  | 2.45                     | 0.51              |
| 52:3:32:A:H2'     | 52:3:33:A:H8     | 1.74                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 52:3:220:G:O2'    | 52:3:221:C:H5'   | 2.11                     | 0.51              |
| 52:3:235:C:H2'    | 52:3:236:A:C8    | 2.46                     | 0.51              |
| 53:1:1229:C:H2'   | 53:1:1230:A:H8   | 1.76                     | 0.51              |
| 53:1:2196:C:O2'   | 53:1:2197:U:H5'  | 2.10                     | 0.51              |
| 7:h:40:GLU:O      | 7:h:43:LYS:HB3   | 2.10                     | 0.51              |
| 26:B:8:THR:CG2    | 53:1:2020:A:H5'  | 2.40                     | 0.51              |
| 31:G:46:VAL:HG23  | 31:G:47:PRO:HD3  | 1.92                     | 0.51              |
| 36:L:71:THR:HG23  | 36:L:72:VAL:HG12 | 1.92                     | 0.51              |
| 46:V:29:LYS:HD2   | 46:V:34:GLY:HA2  | 1.93                     | 0.51              |
| 51:a:189:LEU:HD12 | 51:a:190:GLU:N   | 2.26                     | 0.51              |
| 53:1:302:C:H2'    | 53:1:303:G:H8    | 1.76                     | 0.51              |
| 53:1:523:C:H2'    | 53:1:524:G:C8    | 2.45                     | 0.51              |
| 53:1:1316:U:H2'   | 53:1:1317:G:C8   | 2.46                     | 0.51              |
| 53:1:2443:C:O2'   | 53:1:2444:G:H5'  | 2.11                     | 0.51              |
| 55:6:51:C:H2'     | 55:6:52:G:H8     | 1.76                     | 0.51              |
| 11:l:82:LEU:HD23  | 11:l:82:LEU:O    | 2.11                     | 0.51              |
| 46:V:64:ARG:O     | 46:V:66:LEU:HG   | 2.09                     | 0.51              |
| 52:3:477:C:H2'    | 52:3:478:A:C8    | 2.45                     | 0.51              |
| 52:3:600:A:H2'    | 52:3:601:G:C8    | 2.46                     | 0.51              |
| 52:3:715:A:H2'    | 52:3:716:A:C8    | 2.46                     | 0.51              |
| 53:1:821:A:H5''   | 53:1:822:G:H5''  | 1.92                     | 0.51              |
| 53:1:1611:C:H6    | 53:1:1611:C:H5'  | 1.75                     | 0.51              |
| 9:j:117:ALA:HA    | 9:j:120:ARG:HH21 | 1.76                     | 0.51              |
| 19:t:51:PHE:O     | 19:t:52:GLU:HG3  | 2.10                     | 0.51              |
| 30:F:1:MET:N      | 53:1:2526:G:N3   | 2.59                     | 0.51              |
| 32:H:78:LYS:HZ3   | 32:H:79:LYS:HB2  | 1.76                     | 0.51              |
| 33:I:127:ARG:HH21 | 52:3:619:U:H4'   | 1.76                     | 0.51              |
| 38:N:99:LYS:NZ    | 52:3:1176:A:OP1  | 2.44                     | 0.51              |
| 51:a:7:ARG:HH21   | 51:a:7:ARG:HG3   | 1.75                     | 0.51              |
| 53:1:1083:U:H2'   | 53:1:1085:A:OP2  | 2.10                     | 0.51              |
| 53:1:1495:A:H2    | 53:1:1578:U:H1'  | 1.76                     | 0.51              |
| 1:b:114:GLN:NE2   | 1:b:115:ILE:O    | 2.44                     | 0.50              |
| 7:h:6:GLN:O       | 7:h:9:GLN:HG3    | 2.10                     | 0.50              |
| 11:l:9:ALA:HB3    | 11:l:12:SER:HB2  | 1.93                     | 0.50              |
| 11:l:30:THR:HG22  | 53:1:810:U:O4    | 2.11                     | 0.50              |
| 12:m:69:PRO:O     | 12:m:70:ASP:OD2  | 2.30                     | 0.50              |
| 38:N:105:ARG:HD2  | 52:3:1117:A:O2'  | 2.12                     | 0.50              |
| 47:W:48:ALA:HB2   | 52:3:834:U:OP1   | 2.11                     | 0.50              |
| 52:3:181:A:N6     | 52:3:194:C:H2'   | 2.26                     | 0.50              |
| 53:1:1550:C:H2'   | 53:1:1551:A:H8   | 1.75                     | 0.50              |
| 53:1:2066:C:O2'   | 53:1:2067:G:H5'  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:k:7:MET:HB3   | 10:k:18:ARG:HD2  | 1.92                     | 0.50              |
| 11:l:3:LEU:HD23  | 53:1:1203:U:C4'  | 2.40                     | 0.50              |
| 11:l:30:THR:O    | 11:l:33:ARG:HG2  | 2.11                     | 0.50              |
| 14:o:53:THR:HG22 | 14:o:65:THR:HB   | 1.93                     | 0.50              |
| 15:p:38:ARG:HH11 | 52:3:345:C:H5'   | 1.76                     | 0.50              |
| 21:v:9:ARG:HG2   | 21:v:41:GLU:HB3  | 1.92                     | 0.50              |
| 27:C:16:THR:HB   | 27:C:41:VAL:HG21 | 1.92                     | 0.50              |
| 49:Y:55:PRO:HB3  | 52:3:193:C:O3'   | 2.11                     | 0.50              |
| 52:3:321:A:H2'   | 52:3:322:C:C6    | 2.45                     | 0.50              |
| 53:1:1287:A:O2'  | 53:1:1288:G:H5'  | 2.12                     | 0.50              |
| 53:1:1987:A:H2'  | 53:1:1988:G:H8   | 1.76                     | 0.50              |
| 58:8:349:GLU:HG3 | 58:8:350:MET:HG3 | 1.92                     | 0.50              |
| 7:h:31:ARG:HE    | 53:1:1054:A:H4'  | 1.76                     | 0.50              |
| 11:l:63:LYS:HE2  | 53:1:2394:C:H5'' | 1.92                     | 0.50              |
| 12:m:17:ASN:HD22 | 12:m:95:LEU:HD22 | 1.76                     | 0.50              |
| 16:q:30:VAL:HG13 | 53:1:580:U:O3'   | 2.11                     | 0.50              |
| 46:V:45:VAL:HG13 | 46:V:73:THR:HA   | 1.94                     | 0.50              |
| 48:X:14:LEU:HD13 | 48:X:32:THR:HG21 | 1.93                     | 0.50              |
| 48:X:31:ARG:HD3  | 48:X:56:HIS:CD2  | 2.46                     | 0.50              |
| 53:1:251:A:H2'   | 53:1:252:G:O4'   | 2.10                     | 0.50              |
| 53:1:395:U:H2'   | 53:1:396:G:C8    | 2.47                     | 0.50              |
| 53:1:598:U:H2'   | 53:1:599:A:H8    | 1.76                     | 0.50              |
| 53:1:2515:C:H2'  | 53:1:2516:A:C8   | 2.47                     | 0.50              |
| 53:1:2795:C:H2'  | 53:1:2796:U:O4'  | 2.12                     | 0.50              |
| 53:1:2860:A:H2'  | 53:1:2861:U:H5'  | 1.93                     | 0.50              |
| 7:h:28:ALA:HB3   | 7:h:109:LYS:HE3  | 1.93                     | 0.50              |
| 9:j:109:LEU:HD22 | 9:j:118:MET:HE2  | 1.93                     | 0.50              |
| 34:J:87:VAL:HA   | 34:J:91:SER:O    | 2.12                     | 0.50              |
| 34:J:107:GLY:CA  | 52:3:9:G:H5'     | 2.40                     | 0.50              |
| 52:3:1330:U:H2'  | 52:3:1331:G:O4'  | 2.11                     | 0.50              |
| 53:1:151:C:H2'   | 53:1:152:A:H8    | 1.76                     | 0.50              |
| 53:1:189:G:H2'   | 53:1:205:G:H22   | 1.76                     | 0.50              |
| 31:G:209:VAL:HA  | 31:G:212:TYR:CD2 | 2.46                     | 0.50              |
| 43:S:63:CYS:HB3  | 43:S:67:GLY:H    | 1.76                     | 0.50              |
| 52:3:405:U:C3'   | 52:3:406:G:H5'   | 2.35                     | 0.50              |
| 52:3:576:C:OP2   | 52:3:577:G:H5''  | 2.12                     | 0.50              |
| 53:1:176:A:O2'   | 53:1:177:G:H5'   | 2.12                     | 0.50              |
| 53:1:293:U:H3'   | 53:1:294:A:H5''  | 1.93                     | 0.50              |
| 53:1:1330:C:O2'  | 53:1:1331:G:H5'  | 2.11                     | 0.50              |
| 54:2:19:C:H2'    | 54:2:20:G:C8     | 2.46                     | 0.50              |
| 54:2:51:G:H2'    | 54:2:52:A:O4'    | 2.12                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 54:2:88:C:H4'     | 54:2:89:U:OP1    | 2.11                     | 0.50              |
| 58:8:141:VAL:HG13 | 58:8:141:VAL:O   | 2.11                     | 0.50              |
| 3:d:143:LEU:HD22  | 3:d:185:LYS:HG3  | 1.94                     | 0.50              |
| 7:h:3:LEU:O       | 7:h:6:GLN:HG3    | 2.10                     | 0.50              |
| 32:H:38:VAL:O     | 32:H:42:LEU:HD23 | 2.11                     | 0.50              |
| 43:S:4:SER:HB3    | 52:3:1216:A:H5'' | 1.94                     | 0.50              |
| 49:Y:73:ARG:HG2   | 49:Y:77:ASN:HD22 | 1.77                     | 0.50              |
| 52:3:758:C:H4'    | 52:3:880:C:H4'   | 1.92                     | 0.50              |
| 52:3:1298:U:H4'   | 52:3:1299:A:O4'  | 2.11                     | 0.50              |
| 53:1:250:G:C6     | 53:1:251:A:C6    | 3.00                     | 0.50              |
| 53:1:572:A:H5''   | 53:1:573:U:OP2   | 2.11                     | 0.50              |
| 53:1:1373:A:H5'   | 53:1:2212:A:H1'  | 1.94                     | 0.50              |
| 53:1:2224:G:H4'   | 53:1:2226:C:C2   | 2.47                     | 0.50              |
| 2:c:61:THR:OG1    | 2:c:63:PRO:HD2   | 2.12                     | 0.50              |
| 51:a:221:GLY:N    | 53:1:2176:A:H5'' | 2.27                     | 0.50              |
| 52:3:1256:A:O2'   | 52:3:1257:A:H5'' | 2.11                     | 0.50              |
| 53:1:2773:C:H2'   | 53:1:2774:C:C6   | 2.46                     | 0.50              |
| 58:8:325:LYS:HZ1  | 58:8:349:GLU:HA  | 1.76                     | 0.50              |
| 3:d:24:ASN:ND2    | 3:d:27:LEU:HB2   | 2.27                     | 0.50              |
| 3:d:181:ILE:HG23  | 11:l:2:ARG:HB3   | 1.94                     | 0.50              |
| 7:h:37:LYS:HE2    | 53:1:1084:A:H62  | 1.76                     | 0.50              |
| 18:s:83:LYS:NZ    | 53:1:1260:A:OP1  | 2.44                     | 0.50              |
| 35:K:46:GLN:HA    | 35:K:56:LYS:HG2  | 1.93                     | 0.50              |
| 38:N:104:THR:HG22 | 38:N:106:ASP:H   | 1.76                     | 0.50              |
| 46:V:10:ARG:O     | 46:V:22:VAL:HG23 | 2.12                     | 0.50              |
| 52:3:49:U:O2'     | 52:3:50:A:H2'    | 2.12                     | 0.50              |
| 52:3:211:G:C2'    | 52:3:212:G:H5'   | 2.41                     | 0.50              |
| 52:3:889:A:H5'    | 52:3:891:U:H1'   | 1.94                     | 0.50              |
| 53:1:340:A:H2'    | 53:1:341:C:O4'   | 2.11                     | 0.50              |
| 53:1:2176:A:H2'   | 53:1:2177:C:C6   | 2.47                     | 0.50              |
| 53:1:2238:G:H2'   | 53:1:2238:G:N3   | 2.27                     | 0.50              |
| 55:5:62:C:H2'     | 55:5:63:G:H8     | 1.77                     | 0.50              |
| 2:c:97:SER:OG     | 2:c:98:VAL:N     | 2.45                     | 0.50              |
| 14:o:53:THR:CG2   | 14:o:65:THR:HB   | 2.42                     | 0.50              |
| 43:S:81:ILE:HG21  | 52:3:1202:U:N3   | 2.26                     | 0.50              |
| 51:a:181:ASP:HB3  | 51:a:184:LYS:HG2 | 1.94                     | 0.50              |
| 52:3:82:G:H2'     | 52:3:83:C:H5'    | 1.94                     | 0.50              |
| 53:1:383:C:H5''   | 53:1:385:C:OP2   | 2.12                     | 0.50              |
| 53:1:616:A:H2'    | 53:1:617:G:O4'   | 2.12                     | 0.50              |
| 53:1:750:A:H2'    | 53:1:751:A:H5''  | 1.94                     | 0.50              |
| 53:1:1965:C:H5''  | 53:1:1966:A:H2'  | 1.93                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:2498:C:O2'  | 53:1:2499:C:H5'   | 2.12                     | 0.50              |
| 54:2:19:C:H2'    | 54:2:20:G:H8      | 1.77                     | 0.50              |
| 55:6:21:A:O2'    | 55:6:22:G:C8      | 2.65                     | 0.50              |
| 12:m:40:ARG:HH11 | 12:m:93:VAL:HG11  | 1.77                     | 0.49              |
| 23:x:18:SER:OG   | 53:1:2080:A:H5'   | 2.11                     | 0.49              |
| 32:H:86:LEU:HA   | 32:H:89:VAL:HG12  | 1.93                     | 0.49              |
| 34:J:114:LEU:O   | 34:J:119:VAL:HG22 | 2.12                     | 0.49              |
| 48:X:39:ILE:HB   | 48:X:66:VAL:HA    | 1.94                     | 0.49              |
| 50:Z:11:PHE:C    | 50:Z:13:VAL:H     | 2.20                     | 0.49              |
| 52:3:1199:U:H2'  | 52:3:1200:C:H5'   | 1.93                     | 0.49              |
| 52:3:1288:A:O2'  | 52:3:1353:G:H5'   | 2.12                     | 0.49              |
| 53:1:738:G:H1    | 53:1:758:C:H42    | 1.59                     | 0.49              |
| 53:1:1706:C:C2   | 53:1:1757:A:H5'   | 2.46                     | 0.49              |
| 53:1:2398:U:H2'  | 53:1:2399:G:C8    | 2.47                     | 0.49              |
| 1:b:48:ILE:HG23  | 1:b:48:ILE:O      | 2.12                     | 0.49              |
| 27:C:20:TYR:OH   | 53:1:2348:U:H5'   | 2.12                     | 0.49              |
| 28:D:12:ARG:NH2  | 53:1:686:U:O4     | 2.45                     | 0.49              |
| 35:K:79:ARG:NH1  | 35:K:79:ARG:HB2   | 2.26                     | 0.49              |
| 36:L:3:ARG:HH22  | 52:3:932:C:C5'    | 2.24                     | 0.49              |
| 36:L:12:LEU:HD12 | 36:L:13:PRO:HD2   | 1.94                     | 0.49              |
| 41:Q:42:LYS:NZ   | 52:3:912:C:H5''   | 2.27                     | 0.49              |
| 52:3:1219:A:H2'  | 52:3:1220:G:C8    | 2.47                     | 0.49              |
| 53:1:1083:U:O2'  | 53:1:1084:A:H5'   | 2.13                     | 0.49              |
| 53:1:1675:C:H2'  | 53:1:1676:A:O4'   | 2.12                     | 0.49              |
| 53:1:1683:U:H2'  | 53:1:1684:G:C8    | 2.47                     | 0.49              |
| 53:1:2193:G:H2'  | 53:1:2194:U:C6    | 2.46                     | 0.49              |
| 53:1:2533:U:H2'  | 53:1:2534:A:O4'   | 2.12                     | 0.49              |
| 54:2:118:C:H2'   | 54:2:119:A:H8     | 1.76                     | 0.49              |
| 58:8:20:HIS:CD2  | 58:8:115:GLN:HB3  | 2.47                     | 0.49              |
| 2:c:25:THR:HG21  | 2:c:193:VAL:HG22  | 1.95                     | 0.49              |
| 6:g:133:GLN:NE2  | 6:g:139:PHE:HB3   | 2.27                     | 0.49              |
| 14:o:40:ILE:HG12 | 14:o:47:VAL:HG12  | 1.93                     | 0.49              |
| 32:H:62:SER:OG   | 32:H:97:PRO:HG2   | 2.12                     | 0.49              |
| 52:3:20:U:H2'    | 52:3:21:G:O4'     | 2.12                     | 0.49              |
| 53:1:826:U:H5''  | 53:1:2429:G:P     | 2.53                     | 0.49              |
| 53:1:1103:A:H3'  | 53:1:1104:C:H5''  | 1.95                     | 0.49              |
| 53:1:2691:C:H2'  | 53:1:2692:G:H8    | 1.77                     | 0.49              |
| 54:2:3:C:H42     | 54:2:117:G:H1     | 1.60                     | 0.49              |
| 54:2:106:G:H2'   | 54:2:107:G:O4'    | 2.13                     | 0.49              |
| 58:8:148:GLU:O   | 58:8:152:MET:HG2  | 2.12                     | 0.49              |
| 9:j:2:LYS:HA     | 53:1:995:C:N4     | 2.27                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 28:D:35:ARG:HE   | 53:1:54:G:H1'    | 1.76                     | 0.49              |
| 32:H:114:LEU:O   | 32:H:117:ASP:OD1 | 2.30                     | 0.49              |
| 37:M:28:SER:OG   | 37:M:56:PRO:HB2  | 2.13                     | 0.49              |
| 39:O:57:VAL:O    | 39:O:58:ASN:CB   | 2.59                     | 0.49              |
| 52:3:244:U:O4    | 52:3:906:A:H1'   | 2.12                     | 0.49              |
| 1:b:164:VAL:HG11 | 1:b:180:MET:HE1  | 1.94                     | 0.49              |
| 3:d:15:SER:OG    | 3:d:17:THR:HG22  | 2.13                     | 0.49              |
| 4:e:3:LEU:HA     | 4:e:6:TYR:HB3    | 1.95                     | 0.49              |
| 8:i:116:MET:HG2  | 8:i:117:THR:H    | 1.77                     | 0.49              |
| 19:t:39:THR:O    | 19:t:43:ILE:HG13 | 2.13                     | 0.49              |
| 29:E:6:VAL:HG12  | 29:E:9:ALA:H     | 1.77                     | 0.49              |
| 38:N:121:ARG:NH1 | 52:3:1345:U:OP1  | 2.45                     | 0.49              |
| 40:P:51:PHE:HB3  | 40:P:55:ARG:HB2  | 1.94                     | 0.49              |
| 50:Z:5:VAL:CG1   | 50:Z:19:LYS:HZ3  | 2.24                     | 0.49              |
| 51:a:54:LYS:HD3  | 51:a:57:GLN:NE2  | 2.27                     | 0.49              |
| 53:1:277:G:H4'   | 53:1:278:A:N7    | 2.28                     | 0.49              |
| 53:1:293:U:C3'   | 53:1:294:A:H5''  | 2.42                     | 0.49              |
| 53:1:570:G:H2'   | 53:1:2030:A:N7   | 2.27                     | 0.49              |
| 53:1:872:U:H2'   | 53:1:873:C:C6    | 2.47                     | 0.49              |
| 53:1:1139:G:O2'  | 53:1:1140:C:H5'  | 2.12                     | 0.49              |
| 3:d:21:ARG:HD2   | 3:d:106:LYS:HE2  | 1.95                     | 0.49              |
| 5:f:34:ARG:HG2   | 5:f:74:MET:HE1   | 1.95                     | 0.49              |
| 5:f:87:GLN:NE2   | 5:f:128:THR:O    | 2.45                     | 0.49              |
| 6:g:6:LEU:HD11   | 6:g:37:VAL:HG23  | 1.94                     | 0.49              |
| 7:h:25:ALA:HB3   | 7:h:85:SER:HB2   | 1.95                     | 0.49              |
| 10:k:2:ILE:HG23  | 10:k:6:THR:HG21  | 1.95                     | 0.49              |
| 11:l:23:ILE:HG13 | 17:r:82:HIS:CD2  | 2.47                     | 0.49              |
| 14:o:34:HIS:HA   | 14:o:53:THR:HB   | 1.94                     | 0.49              |
| 24:y:9:LYS:HG3   | 24:y:12:GLU:H    | 1.77                     | 0.49              |
| 24:y:34:SER:OG   | 24:y:36:GLN:HG3  | 2.12                     | 0.49              |
| 27:C:18:HIS:CD2  | 27:C:40:PRO:HG3  | 2.48                     | 0.49              |
| 31:G:13:VAL:HG23 | 31:G:42:LEU:HD21 | 1.94                     | 0.49              |
| 34:J:108:GLY:O   | 34:J:109:ALA:HB3 | 2.12                     | 0.49              |
| 34:J:134:ASN:ND2 | 52:3:19:A:OP1    | 2.45                     | 0.49              |
| 37:M:45:ILE:HD12 | 37:M:45:ILE:N    | 2.27                     | 0.49              |
| 40:P:71:ASP:O    | 40:P:72:ALA:HB3  | 2.12                     | 0.49              |
| 43:S:92:ILE:N    | 43:S:92:ILE:HD12 | 2.27                     | 0.49              |
| 52:3:123:U:H5''  | 52:3:311:C:O2'   | 2.12                     | 0.49              |
| 52:3:711:G:O2'   | 52:3:712:A:H5'   | 2.13                     | 0.49              |
| 52:3:1060:U:H2'  | 52:3:1061:G:C8   | 2.48                     | 0.49              |
| 52:3:1280:A:O2'  | 52:3:1281:C:H5'  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:288:U:H2'   | 53:1:289:G:C8     | 2.48                     | 0.49              |
| 53:1:1181:U:H2'  | 53:1:1182:G:C8    | 2.48                     | 0.49              |
| 53:1:1454:C:H2'  | 53:1:1455:G:H8    | 1.77                     | 0.49              |
| 53:1:2248:C:H2'  | 53:1:2249:U:H5'   | 1.93                     | 0.49              |
| 1:b:206:LYS:HD2  | 53:1:729:G:OP2    | 2.13                     | 0.49              |
| 3:d:144:GLU:HG2  | 3:d:145:ASP:N     | 2.28                     | 0.49              |
| 27:C:46:VAL:HG12 | 27:C:47:ILE:H     | 1.78                     | 0.49              |
| 30:F:17:VAL:HG12 | 30:F:19:ARG:HG3   | 1.95                     | 0.49              |
| 32:H:175:HIS:HE2 | 52:3:1190:G:H5''  | 1.78                     | 0.49              |
| 51:a:60:ARG:HD2  | 51:a:164:ARG:HD3  | 1.94                     | 0.49              |
| 52:3:1120:C:H2'  | 52:3:1121:U:C6    | 2.47                     | 0.49              |
| 52:3:1202:U:H2'  | 52:3:1203:C:H5'   | 1.94                     | 0.49              |
| 53:1:1020:A:C1'  | 53:1:1021:A:OP2   | 2.58                     | 0.49              |
| 53:1:2120:G:H2'  | 53:1:2121:G:H8    | 1.78                     | 0.49              |
| 53:1:2391:G:H5'  | 53:1:2392:A:OP1   | 2.13                     | 0.49              |
| 53:1:2636:C:H2'  | 53:1:2637:U:C6    | 2.47                     | 0.49              |
| 1:b:223:ALA:O    | 53:1:782:A:O2'    | 2.29                     | 0.49              |
| 1:b:242:HIS:O    | 1:b:244:VAL:HG23  | 2.13                     | 0.49              |
| 23:x:16:ASN:HB2  | 23:x:26:ARG:HG2   | 1.95                     | 0.49              |
| 31:G:49:PHE:HD1  | 31:G:199:ILE:HD13 | 1.78                     | 0.49              |
| 36:L:3:ARG:CZ    | 52:3:932:C:H5''   | 2.43                     | 0.49              |
| 36:L:55:LYS:HB2  | 36:L:60:ALA:HB2   | 1.95                     | 0.49              |
| 50:Z:50:SER:HA   | 50:Z:53:LYS:CE    | 2.42                     | 0.49              |
| 51:a:12:ARG:HE   | 51:a:220:ALA:HB2  | 1.78                     | 0.49              |
| 51:a:62:ALA:HB2  | 51:a:162:ARG:NE   | 2.27                     | 0.49              |
| 52:3:9:G:H2'     | 52:3:10:A:H8      | 1.76                     | 0.49              |
| 52:3:730:G:C2'   | 52:3:731:G:H5'    | 2.42                     | 0.49              |
| 52:3:763:G:H2'   | 52:3:764:C:C6     | 2.47                     | 0.49              |
| 53:1:433:C:O2'   | 53:1:434:U:H5'    | 2.13                     | 0.49              |
| 53:1:677:A:O2'   | 53:1:2071:A:H5'   | 2.13                     | 0.49              |
| 53:1:1833:C:H2'  | 53:1:1834:U:O4'   | 2.12                     | 0.49              |
| 53:1:2843:G:O2'  | 53:1:2844:G:H5'   | 2.12                     | 0.49              |
| 55:5:62:C:H2'    | 55:5:63:G:C8      | 2.48                     | 0.49              |
| 58:8:22:ASP:HA   | 61:8:501:GTP:H5'' | 1.93                     | 0.49              |
| 15:p:25:VAL:HG22 | 15:p:26:GLU:H     | 1.76                     | 0.49              |
| 21:v:61:LEU:HD23 | 21:v:62:THR:N     | 2.27                     | 0.49              |
| 29:E:8:GLY:O     | 29:E:12:ARG:NH2   | 2.43                     | 0.49              |
| 39:O:57:VAL:HG22 | 39:O:58:ASN:N     | 2.28                     | 0.49              |
| 40:P:126:ARG:HA  | 40:P:126:ARG:HH11 | 1.77                     | 0.49              |
| 52:3:1512:U:H2'  | 52:3:1513:A:H8    | 1.78                     | 0.49              |
| 53:1:1045:C:H5'  | 53:1:1046:A:H5''  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:e:37:MET:HB3   | 4:e:86:CYS:SG    | 2.52                     | 0.49              |
| 16:q:43:GLN:NE2  | 17:r:77:PHE:O    | 2.46                     | 0.49              |
| 23:x:12:VAL:HG13 | 23:x:28:PHE:HB2  | 1.95                     | 0.49              |
| 32:H:46:LEU:HB3  | 32:H:49:ALA:HB3  | 1.95                     | 0.49              |
| 50:Z:6:ARG:C     | 50:Z:8:ASN:N     | 2.70                     | 0.49              |
| 53:1:230:G:O2'   | 53:1:231:A:H5'   | 2.13                     | 0.49              |
| 53:1:971:G:H2'   | 53:1:972:A:O4'   | 2.13                     | 0.49              |
| 53:1:1344:U:H3'  | 53:1:1345:C:H5'  | 1.94                     | 0.49              |
| 58:8:23:HIS:O    | 58:8:136:ASN:ND2 | 2.45                     | 0.49              |
| 2:c:2:ILE:HG21   | 2:c:90:PHE:HE2   | 1.77                     | 0.48              |
| 3:d:58:LYS:NZ    | 3:d:70:SER:O     | 2.46                     | 0.48              |
| 9:j:84:ILE:HG23  | 9:j:84:ILE:O     | 2.13                     | 0.48              |
| 13:n:38:LEU:HB3  | 13:n:39:PRO:HD3  | 1.94                     | 0.48              |
| 19:t:93:LEU:OXT  | 19:t:93:LEU:HD23 | 2.12                     | 0.48              |
| 32:H:22:PHE:HB2  | 39:O:95:GLY:O    | 2.13                     | 0.48              |
| 33:I:103:ARG:HD2 | 33:I:167:PRO:HG2 | 1.95                     | 0.48              |
| 33:I:205:LYS:HD2 | 52:3:8:A:N6      | 2.29                     | 0.48              |
| 38:N:8:THR:OG1   | 38:N:9:GLY:N     | 2.43                     | 0.48              |
| 43:S:65:GLN:HG3  | 43:S:78:LEU:HD22 | 1.93                     | 0.48              |
| 51:a:54:LYS:HD3  | 51:a:57:GLN:HE21 | 1.78                     | 0.48              |
| 52:3:77:A:H2'    | 52:3:78:A:C8     | 2.48                     | 0.48              |
| 52:3:240:G:H2'   | 52:3:241:G:H8    | 1.78                     | 0.48              |
| 52:3:552:U:H2'   | 52:3:553:A:H8    | 1.78                     | 0.48              |
| 52:3:588:G:H1    | 52:3:651:C:H42   | 1.59                     | 0.48              |
| 52:3:1125:U:H2'  | 52:3:1126:U:H2'  | 1.94                     | 0.48              |
| 53:1:164:C:H2'   | 53:1:165:A:O4'   | 2.12                     | 0.48              |
| 53:1:189:G:H2'   | 53:1:205:G:N2    | 2.28                     | 0.48              |
| 53:1:876:C:H2'   | 53:1:877:A:O4'   | 2.13                     | 0.48              |
| 55:6:35:A:H2'    | 55:6:36:U:C6     | 2.48                     | 0.48              |
| 1:b:158:GLY:N    | 1:b:194:VAL:HG23 | 2.28                     | 0.48              |
| 5:f:154:GLU:HB3  | 5:f:159:LYS:H    | 1.78                     | 0.48              |
| 10:k:70:ARG:HG2  | 10:k:76:VAL:HG12 | 1.94                     | 0.48              |
| 22:w:39:THR:H    | 53:1:2331:G:C4'  | 2.25                     | 0.48              |
| 38:N:6:TYR:CE2   | 52:3:1147:C:H4'  | 2.47                     | 0.48              |
| 52:3:229:U:H2'   | 52:3:230:G:C8    | 2.48                     | 0.48              |
| 52:3:664:G:N2    | 52:3:741:G:H1    | 2.10                     | 0.48              |
| 52:3:744:C:H2'   | 52:3:745:G:C8    | 2.47                     | 0.48              |
| 52:3:1173:U:H2'  | 52:3:1174:G:C8   | 2.48                     | 0.48              |
| 52:3:1496:C:H2'  | 52:3:1497:G:O4'  | 2.13                     | 0.48              |
| 53:1:155:A:H2'   | 53:1:156:A:C8    | 2.48                     | 0.48              |
| 53:1:1268:A:H2'  | 53:1:1269:A:O4'  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:1991:U:C2'  | 53:1:1992:G:H5''  | 2.43                     | 0.48              |
| 57:7:65:G:H2'    | 57:7:66:U:C6      | 2.48                     | 0.48              |
| 58:8:12:HIS:HA   | 58:8:76:HIS:HB3   | 1.95                     | 0.48              |
| 58:8:103:ILE:O   | 58:8:103:ILE:HG13 | 2.12                     | 0.48              |
| 5:f:163:TYR:HB2  | 5:f:166:GLU:CB    | 2.42                     | 0.48              |
| 7:h:23:LEU:HB3   | 7:h:87:GLU:OE1    | 2.13                     | 0.48              |
| 7:h:107:GLU:HG2  | 7:h:110:ALA:HB2   | 1.94                     | 0.48              |
| 10:k:102:PRO:HB3 | 10:k:121:GLU:HB3  | 1.95                     | 0.48              |
| 38:N:74:GLN:O    | 38:N:78:ILE:HG13  | 2.12                     | 0.48              |
| 45:U:63:GLN:NE2  | 52:3:228:A:H5'    | 2.28                     | 0.48              |
| 52:3:202:G:H2'   | 52:3:203:G:C8     | 2.49                     | 0.48              |
| 52:3:794:A:O2'   | 52:3:795:C:H5'    | 2.13                     | 0.48              |
| 52:3:1123:U:O2'  | 52:3:1124:G:H5'   | 2.13                     | 0.48              |
| 52:3:1527:U:H2'  | 52:3:1528:U:C6    | 2.48                     | 0.48              |
| 53:1:1572:A:H2'  | 53:1:1573:G:H8    | 1.77                     | 0.48              |
| 58:8:322:PRO:HB3 | 58:8:352:MET:HA   | 1.95                     | 0.48              |
| 1:b:200:MET:HE3  | 52:3:773:G:H4'    | 1.95                     | 0.48              |
| 11:l:62:PRO:HB2  | 29:E:29:ARG:HH11  | 1.78                     | 0.48              |
| 33:I:143:SER:C   | 33:I:144:ILE:HD12 | 2.38                     | 0.48              |
| 37:M:27:PRO:O    | 37:M:32:LYS:NZ    | 2.47                     | 0.48              |
| 48:X:44:ILE:HD13 | 48:X:63:ASP:HA    | 1.95                     | 0.48              |
| 52:3:701:U:C4'   | 52:3:703:G:H1'    | 2.43                     | 0.48              |
| 53:1:527:C:C4    | 53:1:2779:U:H2'   | 2.48                     | 0.48              |
| 53:1:729:G:H4'   | 53:1:763:G:C5'    | 2.42                     | 0.48              |
| 53:1:1424:G:H2'  | 53:1:1425:G:O4'   | 2.14                     | 0.48              |
| 53:1:1507:C:H2'  | 53:1:1508:A:O4'   | 2.12                     | 0.48              |
| 6:g:66:ASN:ND2   | 6:g:135:HIS:HB2   | 2.28                     | 0.48              |
| 11:l:59:ARG:HD2  | 53:1:250:G:H4'    | 1.96                     | 0.48              |
| 12:m:4:PRO:HG3   | 12:m:68:PHE:HE2   | 1.77                     | 0.48              |
| 43:S:5:MET:SD    | 43:S:8:ARG:NH2    | 2.87                     | 0.48              |
| 52:3:410:G:H2'   | 52:3:429:U:C4     | 2.48                     | 0.48              |
| 52:3:526:C:H3'   | 52:3:527:G:C5'    | 2.43                     | 0.48              |
| 52:3:530:G:H3'   | 52:3:531:U:C5'    | 2.44                     | 0.48              |
| 52:3:1148:U:H2'  | 52:3:1149:C:O4'   | 2.13                     | 0.48              |
| 53:1:414:C:H2'   | 53:1:415:A:C8     | 2.49                     | 0.48              |
| 53:1:1700:A:H2'  | 53:1:1701:A:H5'   | 1.95                     | 0.48              |
| 53:1:2520:C:O2'  | 53:1:2521:C:H5'   | 2.14                     | 0.48              |
| 53:1:2538:C:H2'  | 53:1:2539:C:C6    | 2.47                     | 0.48              |
| 56:4:19:U:H2'    | 56:4:20:U:C6      | 2.48                     | 0.48              |
| 58:8:28:LEU:O    | 58:8:32:ILE:HG13  | 2.13                     | 0.48              |
| 1:b:233:GLY:HA3  | 53:1:2598:A:H5''  | 1.96                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:c:53:GLY:HA3   | 2:c:77:ARG:HG2    | 1.95                     | 0.48              |
| 11:l:93:ASN:C    | 11:l:95:LEU:H     | 2.21                     | 0.48              |
| 17:r:39:LEU:O    | 17:r:49:ILE:HG23  | 2.14                     | 0.48              |
| 22:w:33:ILE:HD11 | 22:w:78:ILE:HD11  | 1.96                     | 0.48              |
| 34:J:79:THR:OG1  | 34:J:80:LEU:N     | 2.47                     | 0.48              |
| 38:N:57:VAL:HG22 | 38:N:59:LYS:NZ    | 2.27                     | 0.48              |
| 52:3:130:A:O2'   | 52:3:264:C:H5'    | 2.14                     | 0.48              |
| 52:3:371:A:H2'   | 52:3:372:C:O4'    | 2.14                     | 0.48              |
| 53:1:851:C:H2'   | 53:1:852:U:C6     | 2.49                     | 0.48              |
| 53:1:1478:G:O2'  | 53:1:1479:G:H5'   | 2.13                     | 0.48              |
| 58:8:308:GLU:OE2 | 58:8:358:LYS:HB3  | 2.13                     | 0.48              |
| 58:8:313:SER:H   | 58:8:316:GLU:HB3  | 1.78                     | 0.48              |
| 6:g:78:VAL:HB    | 6:g:144:VAL:HG22  | 1.95                     | 0.48              |
| 15:p:105:LYS:O   | 15:p:108:ARG:HG2  | 2.13                     | 0.48              |
| 17:r:91:GLN:HE21 | 53:1:993:G:H1'    | 1.78                     | 0.48              |
| 19:t:8:LEU:HD23  | 19:t:50:LEU:HD21  | 1.95                     | 0.48              |
| 32:H:78:LYS:HB3  | 32:H:81:GLU:OE1   | 2.14                     | 0.48              |
| 38:N:119:LYS:O   | 38:N:120:ALA:HB3  | 2.14                     | 0.48              |
| 52:3:715:A:H2'   | 52:3:716:A:H8     | 1.79                     | 0.48              |
| 52:3:736:C:H2'   | 52:3:737:C:C6     | 2.49                     | 0.48              |
| 52:3:1386:G:H2'  | 52:3:1387:G:H8    | 1.79                     | 0.48              |
| 53:1:372:G:HO2'  | 53:1:373:U:H5     | 1.59                     | 0.48              |
| 53:1:906:U:C3'   | 53:1:907:G:H5''   | 2.44                     | 0.48              |
| 53:1:2746:U:O4   | 53:1:2755:C:H4'   | 2.13                     | 0.48              |
| 58:8:207:ILE:HB  | 58:8:236:ILE:HG23 | 1.96                     | 0.48              |
| 6:g:37:VAL:HG12  | 6:g:43:ASN:HD22   | 1.78                     | 0.48              |
| 8:i:33:ASN:HB3   | 8:i:35:MET:HG2    | 1.95                     | 0.48              |
| 9:j:68:LYS:HD3   | 53:1:1022:G:N7    | 2.29                     | 0.48              |
| 20:u:34:ILE:CD1  | 20:u:63:ALA:HB2   | 2.44                     | 0.48              |
| 25:z:10:ARG:HB2  | 25:z:10:ARG:HH21  | 1.76                     | 0.48              |
| 28:D:12:ARG:HE   | 28:D:44:VAL:CG2   | 2.21                     | 0.48              |
| 33:I:167:PRO:HB2 | 33:I:170:LEU:CD2  | 2.44                     | 0.48              |
| 35:K:69:GLU:O    | 35:K:73:GLU:HG2   | 2.13                     | 0.48              |
| 39:O:41:PRO:HB3  | 52:3:1151:A:H1'   | 1.96                     | 0.48              |
| 40:P:30:ILE:HG12 | 40:P:45:THR:HG22  | 1.96                     | 0.48              |
| 47:W:33:THR:HG23 | 47:W:35:SER:H     | 1.79                     | 0.48              |
| 52:3:12:U:H2'    | 52:3:13:U:H5''    | 1.94                     | 0.48              |
| 52:3:864:A:H2'   | 52:3:865:A:C8     | 2.49                     | 0.48              |
| 53:1:37:C:H4'    | 53:1:451:U:OP1    | 2.14                     | 0.48              |
| 53:1:2489:U:O2'  | 53:1:2490:G:H5'   | 2.13                     | 0.48              |
| 53:1:2579:C:O2'  | 53:1:2580:U:H5'   | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:2743:U:H3'   | 53:1:2744:G:H5''  | 1.95                     | 0.48              |
| 2:c:148:GLN:OE1   | 2:c:148:GLN:N     | 2.46                     | 0.48              |
| 10:k:40:LYS:HD3   | 53:1:2562:U:OP1   | 2.13                     | 0.48              |
| 12:m:67:VAL:HG11  | 12:m:102:LEU:HD23 | 1.95                     | 0.48              |
| 21:v:14:LYS:HB2   | 54:2:98:G:H1      | 1.79                     | 0.48              |
| 38:N:17:ARG:HH12  | 52:3:1129:C:H4'   | 1.78                     | 0.48              |
| 38:N:82:ILE:O     | 38:N:86:LEU:HG    | 2.14                     | 0.48              |
| 42:R:78:ARG:O     | 42:R:81:ASP:OD1   | 2.32                     | 0.48              |
| 47:W:13:THR:OG1   | 47:W:18:GLN:N     | 2.47                     | 0.48              |
| 52:3:396:C:C3'    | 52:3:397:A:H5''   | 2.44                     | 0.48              |
| 52:3:525:C:H2'    | 52:3:526:C:C6     | 2.49                     | 0.48              |
| 52:3:1512:U:H2'   | 52:3:1513:A:C8    | 2.49                     | 0.48              |
| 53:1:20:C:H2'     | 53:1:21:A:C8      | 2.49                     | 0.48              |
| 53:1:239:C:H2'    | 53:1:240:C:O4'    | 2.13                     | 0.48              |
| 53:1:381:G:H2'    | 53:1:382:A:C8     | 2.48                     | 0.48              |
| 53:1:2376:A:H2'   | 53:1:2377:A:O4'   | 2.13                     | 0.48              |
| 53:1:2818:U:H2'   | 53:1:2819:G:H8    | 1.79                     | 0.48              |
| 58:8:50:ILE:HG23  | 58:8:66:SER:HB3   | 1.95                     | 0.48              |
| 6:g:66:ASN:ND2    | 6:g:134:VAL:HG13  | 2.28                     | 0.48              |
| 25:z:52:PHE:CD2   | 54:2:83:G:H4'     | 2.49                     | 0.48              |
| 31:G:103:TRP:HE1  | 31:G:107:ARG:HH21 | 1.61                     | 0.48              |
| 34:J:104:ILE:HG23 | 34:J:111:ARG:HH12 | 1.79                     | 0.48              |
| 47:W:59:LYS:HD3   | 52:3:734:G:O2'    | 2.14                     | 0.48              |
| 52:3:89:U:H2'     | 52:3:90:C:O4'     | 2.14                     | 0.48              |
| 52:3:1499:A:O2'   | 52:3:1520:C:H5'   | 2.14                     | 0.48              |
| 53:1:827:U:H4'    | 53:1:828:U:C5     | 2.49                     | 0.48              |
| 53:1:1105:U:C2'   | 53:1:1106:G:H5''  | 2.43                     | 0.48              |
| 53:1:1316:U:H2'   | 53:1:1317:G:H8    | 1.78                     | 0.48              |
| 53:1:1447:C:H2'   | 53:1:1448:G:H8    | 1.78                     | 0.48              |
| 53:1:2339:C:H2'   | 53:1:2340:A:C8    | 2.49                     | 0.48              |
| 58:8:220:SER:HB2  | 58:8:284:ARG:HD3  | 1.95                     | 0.48              |
| 6:g:112:LYS:HZ1   | 53:1:2220:U:C3'   | 2.27                     | 0.47              |
| 10:k:91:SER:OG    | 10:k:93:GLN:HG2   | 2.14                     | 0.47              |
| 18:s:24:ILE:HD12  | 18:s:24:ILE:N     | 2.28                     | 0.47              |
| 52:3:401:C:H2'    | 52:3:402:G:H8     | 1.78                     | 0.47              |
| 52:3:832:G:O2'    | 52:3:833:G:H5'    | 2.14                     | 0.47              |
| 52:3:1230:C:H5'   | 55:5:30:G:H5''    | 1.96                     | 0.47              |
| 53:1:65:U:H2'     | 53:1:66:C:C6      | 2.48                     | 0.47              |
| 53:1:112:U:H2'    | 53:1:113:U:H5'    | 1.96                     | 0.47              |
| 53:1:386:G:H3'    | 53:1:387:U:C5'    | 2.44                     | 0.47              |
| 53:1:593:U:H2'    | 53:1:594:U:C6     | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:863:A:H4'    | 54:2:100:G:N2     | 2.29                     | 0.47              |
| 53:1:1287:A:C2'   | 53:1:1288:G:H5'   | 2.44                     | 0.47              |
| 53:1:2327:A:H2'   | 53:1:2328:A:C8    | 2.49                     | 0.47              |
| 53:1:2545:G:C2'   | 53:1:2546:U:H5'   | 2.44                     | 0.47              |
| 58:8:25:LYS:HA    | 58:8:105:VAL:HG21 | 1.96                     | 0.47              |
| 1:b:42:ARG:O      | 53:1:1813:G:H4'   | 2.15                     | 0.47              |
| 6:g:1:MET:HB3     | 6:g:2:GLN:H       | 1.57                     | 0.47              |
| 6:g:8:LYS:O       | 6:g:8:LYS:HG3     | 2.14                     | 0.47              |
| 7:h:111:ALA:O     | 7:h:114:GLU:HG2   | 2.13                     | 0.47              |
| 15:p:64:SER:OG    | 15:p:65:ASN:N     | 2.47                     | 0.47              |
| 16:q:25:GLY:HA2   | 16:q:29:ARG:HH12  | 1.79                     | 0.47              |
| 21:v:51:GLN:OE1   | 21:v:86:LEU:HD11  | 2.13                     | 0.47              |
| 22:w:39:THR:N     | 53:1:2331:G:H4'   | 2.26                     | 0.47              |
| 33:I:144:ILE:HD12 | 33:I:144:ILE:N    | 2.29                     | 0.47              |
| 38:N:123:ARG:O    | 38:N:125:GLN:N    | 2.47                     | 0.47              |
| 48:X:5:LYS:HD3    | 48:X:6:LYS:NZ     | 2.29                     | 0.47              |
| 52:3:704:A:H2'    | 52:3:705:G:O4'    | 2.14                     | 0.47              |
| 52:3:860:A:H2'    | 52:3:861:G:O4'    | 2.14                     | 0.47              |
| 52:3:1404:C:H2'   | 52:3:1405:G:C8    | 2.49                     | 0.47              |
| 52:3:1429:A:H2'   | 52:3:1430:A:C8    | 2.44                     | 0.47              |
| 53:1:1817:G:N2    | 53:1:1818:U:H1'   | 2.30                     | 0.47              |
| 53:1:1827:U:C2'   | 53:1:1828:G:H5'   | 2.44                     | 0.47              |
| 53:1:2343:U:O2'   | 53:1:2344:U:H5'   | 2.15                     | 0.47              |
| 5:f:157:LYS:HB2   | 5:f:159:LYS:HG3   | 1.96                     | 0.47              |
| 7:h:121:SER:OG    | 7:h:122:GLN:N     | 2.46                     | 0.47              |
| 15:p:31:VAL:CG1   | 15:p:40:GLN:HE21  | 2.27                     | 0.47              |
| 21:v:46:LYS:O     | 21:v:50:MET:HG2   | 2.13                     | 0.47              |
| 24:y:21:LEU:HA    | 24:y:25:GLN:HB3   | 1.96                     | 0.47              |
| 40:P:80:ASN:HA    | 40:P:105:ARG:HB3  | 1.95                     | 0.47              |
| 41:Q:24:GLU:O     | 41:Q:25:ALA:HB3   | 2.14                     | 0.47              |
| 50:Z:5:VAL:HG22   | 50:Z:19:LYS:NZ    | 2.29                     | 0.47              |
| 53:1:912:C:O2'    | 53:1:913:U:H5'    | 2.14                     | 0.47              |
| 53:1:1045:C:P     | 53:1:1047:G:H5'   | 2.54                     | 0.47              |
| 53:1:1905:C:O2'   | 53:1:1929:G:H1'   | 2.14                     | 0.47              |
| 3:d:68:ALA:HA     | 53:1:1255:U:C6    | 2.50                     | 0.47              |
| 21:v:35:GLU:OE1   | 21:v:35:GLU:N     | 2.43                     | 0.47              |
| 32:H:56:ILE:HG23  | 32:H:63:ILE:HD11  | 1.96                     | 0.47              |
| 33:I:150:LYS:O    | 33:I:150:LYS:HD2  | 2.15                     | 0.47              |
| 35:K:43:GLY:HA2   | 35:K:58:HIS:CE1   | 2.50                     | 0.47              |
| 40:P:118:ASN:OD1  | 52:3:718:A:H5'    | 2.14                     | 0.47              |
| 46:V:14:ASP:HA    | 46:V:20:ILE:HG13  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 50:Z:39:LYS:O    | 50:Z:43:GLU:N     | 2.41                     | 0.47              |
| 52:3:868:C:H2'   | 52:3:869:G:O4'    | 2.15                     | 0.47              |
| 53:1:255:A:H2'   | 53:1:256:A:O4'    | 2.14                     | 0.47              |
| 53:1:687:C:H6    | 53:1:687:C:H5'    | 1.79                     | 0.47              |
| 53:1:1794:A:H2'  | 53:1:1795:C:C6    | 2.49                     | 0.47              |
| 53:1:2637:U:H2'  | 53:1:2638:G:O4'   | 2.14                     | 0.47              |
| 57:7:6:G:C2'     | 57:7:7:A:H5''     | 2.44                     | 0.47              |
| 58:8:18:ILE:HB   | 58:8:119:HIS:HB3  | 1.94                     | 0.47              |
| 4:e:110:ILE:HB   | 4:e:113:PHE:HB2   | 1.95                     | 0.47              |
| 6:g:26:ALA:HA    | 6:g:30:LEU:HB2    | 1.96                     | 0.47              |
| 7:h:33:VAL:HG12  | 7:h:34:THR:H      | 1.78                     | 0.47              |
| 10:k:22:ILE:HD12 | 53:1:1952:A:C2    | 2.49                     | 0.47              |
| 23:x:66:VAL:O    | 23:x:69:GLU:HB2   | 2.14                     | 0.47              |
| 32:H:3:LYS:HG2   | 52:3:1191:A:OP1   | 2.14                     | 0.47              |
| 38:N:29:ILE:HB   | 38:N:64:ILE:HB    | 1.96                     | 0.47              |
| 39:O:10:LEU:HD23 | 39:O:10:LEU:H     | 1.80                     | 0.47              |
| 52:3:211:G:H2'   | 52:3:212:G:H5'    | 1.95                     | 0.47              |
| 52:3:250:A:H5'   | 52:3:252:U:H1'    | 1.95                     | 0.47              |
| 52:3:883:C:O2'   | 52:3:884:U:H5'    | 2.15                     | 0.47              |
| 52:3:884:U:H4'   | 52:3:885:G:H5''   | 1.96                     | 0.47              |
| 52:3:924:C:H2'   | 52:3:925:G:C8     | 2.50                     | 0.47              |
| 52:3:1128:C:O2'  | 52:3:1129:C:H5'   | 2.14                     | 0.47              |
| 53:1:163:C:H2'   | 53:1:164:C:O4'    | 2.14                     | 0.47              |
| 53:1:492:A:H2'   | 53:1:493:G:O4'    | 2.15                     | 0.47              |
| 53:1:1023:U:H4'  | 53:1:1123:C:OP1   | 2.14                     | 0.47              |
| 58:8:98:GLN:HA   | 58:8:231:ARG:HD3  | 1.95                     | 0.47              |
| 7:h:94:ARG:O     | 7:h:98:GLU:HG3    | 2.14                     | 0.47              |
| 15:p:88:ARG:NH1  | 15:p:114:ASN:OD1  | 2.47                     | 0.47              |
| 18:s:51:LEU:HD13 | 18:s:105:VAL:HG11 | 1.95                     | 0.47              |
| 32:H:122:GLN:HG3 | 32:H:127:VAL:CG1  | 2.43                     | 0.47              |
| 34:J:84:VAL:HG22 | 34:J:85:LYS:O     | 2.15                     | 0.47              |
| 42:R:64:VAL:CG2  | 42:R:65:GLU:H     | 2.20                     | 0.47              |
| 52:3:403:C:O2'   | 52:3:404:G:H5'    | 2.14                     | 0.47              |
| 53:1:856:G:H2'   | 53:1:857:G:C8     | 2.49                     | 0.47              |
| 53:1:859:G:O2'   | 53:1:860:U:C6     | 2.65                     | 0.47              |
| 53:1:1073:A:H2'  | 53:1:1074:G:O4'   | 2.15                     | 0.47              |
| 2:c:138:LEU:N    | 2:c:138:LEU:HD12  | 2.30                     | 0.47              |
| 21:v:20:LEU:HD23 | 21:v:25:LYS:O     | 2.14                     | 0.47              |
| 23:x:56:ARG:HB3  | 53:1:372:G:N7     | 2.29                     | 0.47              |
| 35:K:5:GLU:HA    | 35:K:63:ASN:HA    | 1.96                     | 0.47              |
| 37:M:112:ASP:N   | 37:M:112:ASP:OD1  | 2.47                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:O:41:PRO:HG3   | 52:3:1150:A:H2    | 1.79                     | 0.47              |
| 39:O:90:LEU:O     | 39:O:90:LEU:HD23  | 2.15                     | 0.47              |
| 43:S:30:ILE:O     | 43:S:30:ILE:HG13  | 2.13                     | 0.47              |
| 46:V:62:GLU:H     | 46:V:62:GLU:CD    | 2.22                     | 0.47              |
| 48:X:54:ARG:HD3   | 52:3:958:A:C4     | 2.49                     | 0.47              |
| 51:a:170:ILE:C    | 51:a:171:ILE:HD12 | 2.39                     | 0.47              |
| 52:3:1435:G:H2'   | 52:3:1436:U:C6    | 2.49                     | 0.47              |
| 52:3:1506:U:O2'   | 52:3:1507:A:H5'   | 2.15                     | 0.47              |
| 53:1:145:C:H2'    | 53:1:146:A:C8     | 2.49                     | 0.47              |
| 53:1:1683:U:H2'   | 53:1:1684:G:H8    | 1.79                     | 0.47              |
| 53:1:1909:C:H2'   | 53:1:1910:G:C8    | 2.47                     | 0.47              |
| 53:1:2217:G:O2'   | 53:1:2218:G:H5'   | 2.15                     | 0.47              |
| 53:1:2221:G:O2'   | 53:1:2222:C:H5'   | 2.15                     | 0.47              |
| 53:1:2297:A:N6    | 53:1:2319:G:H1'   | 2.29                     | 0.47              |
| 53:1:2529:G:OP2   | 53:1:2530:A:H5''  | 2.14                     | 0.47              |
| 53:1:2650:U:H2'   | 53:1:2651:C:C6    | 2.49                     | 0.47              |
| 58:8:67:HIS:HE1   | 58:8:98:GLN:HE22  | 1.63                     | 0.47              |
| 58:8:135:LEU:HB2  | 58:8:172:ARG:HA   | 1.96                     | 0.47              |
| 58:8:183:ALA:HA   | 58:8:186:GLU:HB2  | 1.97                     | 0.47              |
| 2:c:14:ILE:HB     | 2:c:22:ILE:HD11   | 1.96                     | 0.47              |
| 13:n:47:VAL:C     | 13:n:50:PRO:HD2   | 2.40                     | 0.47              |
| 17:r:1:MET:H1     | 17:r:43:ASN:HA    | 1.80                     | 0.47              |
| 27:C:43:ARG:NH2   | 53:1:643:A:H1'    | 2.30                     | 0.47              |
| 31:G:216:VAL:O    | 31:G:220:VAL:HG23 | 2.15                     | 0.47              |
| 31:G:220:VAL:O    | 31:G:224:ARG:HG2  | 2.14                     | 0.47              |
| 34:J:24:VAL:HG12  | 34:J:25:LYS:H     | 1.79                     | 0.47              |
| 34:J:123:LEU:HD22 | 52:3:7:A:H2'      | 1.95                     | 0.47              |
| 45:U:5:ARG:NH2    | 45:U:23:ASP:O     | 2.48                     | 0.47              |
| 50:Z:34:ARG:HB3   | 50:Z:36:PHE:CE2   | 2.50                     | 0.47              |
| 52:3:354:G:H2'    | 52:3:355:C:H5'    | 1.95                     | 0.47              |
| 52:3:1339:A:C2'   | 52:3:1340:A:H5'   | 2.44                     | 0.47              |
| 52:3:1412:C:H2'   | 52:3:1413:A:H8    | 1.79                     | 0.47              |
| 52:3:1464:U:H2'   | 52:3:1465:A:C8    | 2.50                     | 0.47              |
| 53:1:1844:C:H2'   | 53:1:1845:G:C8    | 2.50                     | 0.47              |
| 53:1:1900:A:H1'   | 53:1:1970:A:H2'   | 1.96                     | 0.47              |
| 53:1:2314:A:H2'   | 53:1:2315:G:C8    | 2.50                     | 0.47              |
| 55:5:47:U:H3'     | 55:5:48:C:C5'     | 2.44                     | 0.47              |
| 8:i:129:GLU:HB3   | 8:i:139:VAL:HG11  | 1.97                     | 0.47              |
| 13:n:65:LEU:O     | 13:n:69:ARG:HG2   | 2.15                     | 0.47              |
| 17:r:1:MET:N      | 17:r:43:ASN:HA    | 2.29                     | 0.47              |
| 26:B:14:MET:HG2   | 53:1:15:G:O2'     | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:H:168:ARG:HD2  | 32:H:168:ARG:C    | 2.40                     | 0.47              |
| 32:H:171:ARG:CG   | 52:3:1106:G:H5''  | 2.42                     | 0.47              |
| 33:I:57:LYS:HG3   | 33:I:199:ILE:HG23 | 1.97                     | 0.47              |
| 40:P:88:PRO:HG3   | 50:Z:28:LEU:CD2   | 2.44                     | 0.47              |
| 41:Q:24:GLU:H     | 41:Q:24:GLU:CD    | 2.22                     | 0.47              |
| 50:Z:50:SER:O     | 50:Z:53:LYS:HG2   | 2.15                     | 0.47              |
| 50:Z:64:ALA:HB1   | 50:Z:66:ARG:NH2   | 2.29                     | 0.47              |
| 52:3:1202:U:C2'   | 52:3:1203:C:H5'   | 2.45                     | 0.47              |
| 53:1:704:G:H2'    | 53:1:726:G:H22    | 1.79                     | 0.47              |
| 53:1:979:A:H2'    | 53:1:982:C:H42    | 1.80                     | 0.47              |
| 53:1:2087:G:H2'   | 53:1:2088:A:H8    | 1.80                     | 0.47              |
| 55:5:51:C:H2'     | 55:5:52:G:C8      | 2.50                     | 0.47              |
| 1:b:166:ARG:HG3   | 1:b:171:VAL:HG22  | 1.96                     | 0.47              |
| 7:h:48:ALA:HB3    | 7:h:51:TYR:HE1    | 1.76                     | 0.47              |
| 20:u:82:VAL:HG12  | 20:u:83:GLY:N     | 2.30                     | 0.47              |
| 28:D:21:ARG:NH1   | 53:1:466:A:H5'    | 2.30                     | 0.47              |
| 34:J:20:VAL:HG23  | 34:J:31:SER:HB2   | 1.96                     | 0.47              |
| 37:M:100:ILE:HG13 | 37:M:128:VAL:HB   | 1.97                     | 0.47              |
| 40:P:43:TRP:HZ2   | 52:3:686:U:H1'    | 1.79                     | 0.47              |
| 42:R:80:MET:O     | 42:R:91:ARG:NH2   | 2.42                     | 0.47              |
| 43:S:33:VAL:O     | 43:S:33:VAL:HG22  | 2.15                     | 0.47              |
| 47:W:56:ARG:HD2   | 47:W:60:ARG:HH21  | 1.80                     | 0.47              |
| 52:3:16:A:O2'     | 52:3:17:U:H5'     | 2.15                     | 0.47              |
| 52:3:367:U:H5'    | 58:8:280:ARG:NH2  | 2.30                     | 0.47              |
| 52:3:648:A:H2'    | 52:3:649:A:C8     | 2.49                     | 0.47              |
| 52:3:869:G:H4'    | 52:3:872:A:C8     | 2.49                     | 0.47              |
| 52:3:987:G:H2'    | 52:3:988:G:C8     | 2.50                     | 0.47              |
| 52:3:1315:U:H2'   | 52:3:1316:G:O4'   | 2.15                     | 0.47              |
| 53:1:207:A:H2'    | 53:1:208:C:O4'    | 2.15                     | 0.47              |
| 53:1:1229:C:H2'   | 53:1:1230:A:C8    | 2.49                     | 0.47              |
| 53:1:1361:G:H2'   | 53:1:1362:C:C6    | 2.50                     | 0.47              |
| 53:1:1565:C:O2'   | 53:1:1566:A:H2'   | 2.15                     | 0.47              |
| 53:1:1773:A:H2'   | 53:1:1774:C:O4'   | 2.14                     | 0.47              |
| 53:1:2055:C:H5'   | 53:1:2056:G:O5'   | 2.15                     | 0.47              |
| 53:1:2553:G:C3'   | 53:1:2554:U:H5''  | 2.43                     | 0.47              |
| 53:1:2875:C:H2'   | 53:1:2876:G:H8    | 1.81                     | 0.47              |
| 57:7:6:G:H2'      | 57:7:7:A:H5''     | 1.96                     | 0.47              |
| 1:b:199:HIS:CE1   | 1:b:202:ARG:HH21  | 2.33                     | 0.46              |
| 6:g:73:ASN:O      | 6:g:76:GLU:HG3    | 2.15                     | 0.46              |
| 12:m:18:ARG:HG2   | 54:2:90:C:H5'     | 1.96                     | 0.46              |
| 12:m:75:GLU:OE2   | 53:1:957:C:H5'    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:r:18:GLN:HE21  | 17:r:20:VAL:HG22  | 1.80                     | 0.46              |
| 23:x:17:ARG:HE    | 23:x:23:ALA:HB2   | 1.80                     | 0.46              |
| 31:G:124:THR:HA   | 31:G:127:LYS:NZ   | 2.30                     | 0.46              |
| 33:I:32:LYS:HD2   | 52:3:426:U:OP1    | 2.15                     | 0.46              |
| 35:K:12:PRO:O     | 35:K:15:SER:HB3   | 2.15                     | 0.46              |
| 42:R:14:ALA:O     | 42:R:17:ALA:HB3   | 2.15                     | 0.46              |
| 52:3:1390:U:H2'   | 52:3:1391:U:C6    | 2.51                     | 0.46              |
| 53:1:968:C:H2'    | 53:1:969:G:C8     | 2.50                     | 0.46              |
| 53:1:1817:G:C2    | 53:1:1818:U:H1'   | 2.50                     | 0.46              |
| 53:1:1935:G:H1'   | 53:1:1964:G:N2    | 2.29                     | 0.46              |
| 53:1:2029:G:O6    | 53:1:2032:G:H5''  | 2.16                     | 0.46              |
| 53:1:2042:A:H2'   | 53:1:2043:C:H5'   | 1.97                     | 0.46              |
| 53:1:2297:A:H62   | 53:1:2319:G:H1'   | 1.80                     | 0.46              |
| 1:b:156:SER:OG    | 53:1:1818:U:H5'   | 2.15                     | 0.46              |
| 14:o:77:ALA:O     | 14:o:80:GLU:HG3   | 2.16                     | 0.46              |
| 33:I:64:TYR:CE2   | 33:I:93:LEU:HB3   | 2.51                     | 0.46              |
| 34:J:100:GLU:C    | 34:J:102:THR:H    | 2.21                     | 0.46              |
| 40:P:115:ILE:HD12 | 40:P:116:PRO:HD2  | 1.98                     | 0.46              |
| 52:3:9:G:H2'      | 52:3:10:A:C8      | 2.50                     | 0.46              |
| 52:3:204:G:H2'    | 52:3:205:A:C8     | 2.50                     | 0.46              |
| 52:3:858:G:O6     | 52:3:869:G:H3'    | 2.15                     | 0.46              |
| 52:3:880:C:H2'    | 52:3:881:G:C8     | 2.50                     | 0.46              |
| 53:1:141:G:H3'    | 53:1:142:A:O4'    | 2.14                     | 0.46              |
| 53:1:619:G:H3'    | 53:1:620:G:H21    | 1.81                     | 0.46              |
| 53:1:654:A:H3'    | 53:1:654:A:N3     | 2.30                     | 0.46              |
| 53:1:1438:U:O2'   | 53:1:1439:A:H5'   | 2.16                     | 0.46              |
| 53:1:2623:G:H2'   | 53:1:2624:G:C8    | 2.49                     | 0.46              |
| 58:8:99:MET:SD    | 58:8:102:ALA:HB2  | 2.54                     | 0.46              |
| 1:b:16:VAL:HB     | 1:b:203:VAL:HG22  | 1.96                     | 0.46              |
| 27:C:5:ARG:HG2    | 27:C:23:THR:HB    | 1.97                     | 0.46              |
| 30:F:24:ARG:HH22  | 30:F:36:ARG:NH1   | 2.13                     | 0.46              |
| 32:H:80:GLY:O     | 32:H:84:GLU:HG2   | 2.16                     | 0.46              |
| 33:I:101:VAL:HG22 | 33:I:106:PHE:HB2  | 1.96                     | 0.46              |
| 34:J:47:PHE:HZ    | 34:J:137:ARG:HH11 | 1.64                     | 0.46              |
| 34:J:96:GLN:HB3   | 34:J:123:LEU:HB2  | 1.96                     | 0.46              |
| 38:N:48:ARG:O     | 38:N:52:GLU:HG2   | 2.15                     | 0.46              |
| 50:Z:9:GLU:HB3    | 50:Z:10:PRO:CD    | 2.43                     | 0.46              |
| 52:3:709:U:H2'    | 52:3:710:G:C8     | 2.50                     | 0.46              |
| 52:3:1195:C:H2'   | 52:3:1197:A:O4'   | 2.15                     | 0.46              |
| 53:1:873:C:H2'    | 53:1:874:G:C8     | 2.49                     | 0.46              |
| 53:1:2277:G:H2'   | 53:1:2278:A:C5'   | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:2283:C:H2'   | 53:1:2284:A:O4'   | 2.15                     | 0.46              |
| 53:1:2564:A:OP1   | 53:1:2648:G:H4'   | 2.15                     | 0.46              |
| 53:1:2812:G:H2'   | 53:1:2813:A:O4'   | 2.15                     | 0.46              |
| 55:5:29:G:H2'     | 55:5:30:G:H8      | 1.78                     | 0.46              |
| 7:h:34:THR:HG22   | 53:1:1085:A:H61   | 1.80                     | 0.46              |
| 23:x:51:SER:O     | 23:x:55:MET:HG3   | 2.15                     | 0.46              |
| 31:G:114:LYS:HA   | 31:G:117:GLU:OE2  | 2.15                     | 0.46              |
| 32:H:127:VAL:HG22 | 32:H:128:MET:N    | 2.31                     | 0.46              |
| 32:H:153:SER:HB3  | 52:3:1057:G:OP1   | 2.16                     | 0.46              |
| 33:I:40:HIS:CD2   | 33:I:43:ARG:HE    | 2.33                     | 0.46              |
| 33:I:109:THR:HG23 | 33:I:112:GLU:H    | 1.80                     | 0.46              |
| 37:M:11:THR:HG21  | 52:3:876:C:H1'    | 1.98                     | 0.46              |
| 37:M:91:LEU:O     | 37:M:116:ARG:NH2  | 2.47                     | 0.46              |
| 52:3:1411:C:H2'   | 52:3:1412:C:C6    | 2.51                     | 0.46              |
| 52:3:1414:U:H2'   | 52:3:1415:G:C8    | 2.49                     | 0.46              |
| 53:1:45:G:C5'     | 53:1:46:G:H5'     | 2.32                     | 0.46              |
| 53:1:816:C:H2'    | 53:1:817:C:C6     | 2.49                     | 0.46              |
| 53:1:2139:U:H2'   | 53:1:2140:G:C8    | 2.51                     | 0.46              |
| 53:1:2182:U:H2'   | 53:1:2183:A:C8    | 2.50                     | 0.46              |
| 53:1:2233:U:H2'   | 53:1:2234:G:C8    | 2.49                     | 0.46              |
| 56:4:17:U:O2'     | 56:4:18:G:H5'     | 2.15                     | 0.46              |
| 8:i:123:ALA:O     | 8:i:126:ARG:HG2   | 2.16                     | 0.46              |
| 13:n:63:ARG:CZ    | 53:1:1454:C:H5'   | 2.46                     | 0.46              |
| 18:s:6:LYS:HB3    | 18:s:104:THR:HG23 | 1.97                     | 0.46              |
| 20:u:39:ASN:HB3   | 20:u:62:ALA:HB3   | 1.98                     | 0.46              |
| 21:v:48:MET:SD    | 21:v:85:LYS:HA    | 2.55                     | 0.46              |
| 34:J:92:ARG:O     | 34:J:93:VAL:C     | 2.58                     | 0.46              |
| 34:J:104:ILE:HG23 | 34:J:104:ILE:O    | 2.16                     | 0.46              |
| 46:V:32:ILE:HG23  | 46:V:33:TYR:N     | 2.31                     | 0.46              |
| 48:X:72:GLU:OE2   | 52:3:1320:C:H4'   | 2.15                     | 0.46              |
| 50:Z:41:THR:O     | 50:Z:45:LYS:HD3   | 2.15                     | 0.46              |
| 52:3:129:A:H1'    | 52:3:130:A:C8     | 2.50                     | 0.46              |
| 52:3:206:C:H2'    | 52:3:207:C:O4'    | 2.15                     | 0.46              |
| 52:3:524:G:H2'    | 52:3:525:C:C6     | 2.50                     | 0.46              |
| 52:3:1197:A:C2'   | 52:3:1198:G:H5''  | 2.43                     | 0.46              |
| 52:3:1369:C:H2'   | 52:3:1370:G:C8    | 2.50                     | 0.46              |
| 52:3:1473:G:O2'   | 52:3:1474:U:H5'   | 2.16                     | 0.46              |
| 53:1:151:C:H2'    | 53:1:152:A:C8     | 2.51                     | 0.46              |
| 53:1:406:G:H2'    | 53:1:407:G:C8     | 2.50                     | 0.46              |
| 53:1:1571:A:H2'   | 53:1:1572:A:C8    | 2.50                     | 0.46              |
| 53:1:1987:A:H2'   | 53:1:1988:G:C8    | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:2849:U:H4'   | 53:1:2868:A:C2    | 2.50                     | 0.46              |
| 54:2:51:G:O2'     | 54:2:52:A:H5'     | 2.15                     | 0.46              |
| 6:g:72:ILE:HB     | 6:g:108:VAL:HG22  | 1.96                     | 0.46              |
| 18:s:8:ARG:HD3    | 53:1:494:G:OP1    | 2.16                     | 0.46              |
| 20:u:34:ILE:HD13  | 20:u:63:ALA:HB2   | 1.98                     | 0.46              |
| 38:N:24:ASN:HA    | 38:N:58:GLU:OE2   | 2.15                     | 0.46              |
| 38:N:114:LYS:HB2  | 38:N:117:LEU:HD22 | 1.97                     | 0.46              |
| 52:3:148:G:H1     | 52:3:174:A:H61    | 1.64                     | 0.46              |
| 52:3:376:G:O2'    | 52:3:377:G:H5'    | 2.15                     | 0.46              |
| 52:3:1164:G:H2'   | 52:3:1165:U:C6    | 2.49                     | 0.46              |
| 52:3:1305:G:H22   | 52:3:1331:G:H2'   | 1.81                     | 0.46              |
| 53:1:2185:U:H2'   | 53:1:2186:G:C8    | 2.50                     | 0.46              |
| 53:1:2302:U:H2'   | 53:1:2303:G:C8    | 2.51                     | 0.46              |
| 53:1:2358:A:H2'   | 53:1:2359:C:O4'   | 2.16                     | 0.46              |
| 53:1:2514:U:H2'   | 53:1:2515:C:C6    | 2.50                     | 0.46              |
| 53:1:2841:C:H2'   | 53:1:2842:G:C8    | 2.50                     | 0.46              |
| 55:5:69:C:H2'     | 55:5:70:G:H8      | 1.80                     | 0.46              |
| 57:7:18:G:N2      | 57:7:57:G:H2'     | 2.31                     | 0.46              |
| 3:d:6:LYS:HZ1     | 3:d:141:MET:HG2   | 1.81                     | 0.46              |
| 34:J:15:ILE:HD11  | 34:J:37:VAL:HG22  | 1.98                     | 0.46              |
| 35:K:86:ARG:HD3   | 47:W:63:TYR:O     | 2.15                     | 0.46              |
| 49:Y:35:TYR:O     | 49:Y:39:GLU:HG2   | 2.15                     | 0.46              |
| 50:Z:23:GLU:O     | 50:Z:25:ALA:N     | 2.46                     | 0.46              |
| 51:a:5:THR:OG1    | 51:a:6:LYS:N      | 2.48                     | 0.46              |
| 53:1:435:C:C2'    | 53:1:436:C:H5'    | 2.44                     | 0.46              |
| 53:1:974:G:N3     | 53:1:974:G:H2'    | 2.31                     | 0.46              |
| 53:1:1298:C:H2'   | 53:1:1299:G:O4'   | 2.16                     | 0.46              |
| 53:1:1652:A:H2'   | 53:1:1653:G:O4'   | 2.16                     | 0.46              |
| 58:8:307:SER:HA   | 58:8:390:ALA:H    | 1.80                     | 0.46              |
| 14:o:49:VAL:CG1   | 14:o:81:ARG:HG3   | 2.45                     | 0.46              |
| 16:q:57:ARG:NH1   | 16:q:61:ILE:HD11  | 2.31                     | 0.46              |
| 19:t:14:PRO:HA    | 19:t:32:LEU:HB3   | 1.98                     | 0.46              |
| 27:C:24:LYS:HE2   | 27:C:29:LYS:HB2   | 1.97                     | 0.46              |
| 33:I:128:VAL:HG11 | 33:I:145:ARG:HH21 | 1.81                     | 0.46              |
| 52:3:1096:C:H2'   | 52:3:1097:C:C6    | 2.50                     | 0.46              |
| 53:1:406:G:H2'    | 53:1:407:G:H8     | 1.80                     | 0.46              |
| 53:1:738:G:O2'    | 53:1:739:A:H5'    | 2.15                     | 0.46              |
| 53:1:869:G:H2'    | 53:1:870:U:C6     | 2.50                     | 0.46              |
| 53:1:1021:A:H3'   | 53:1:1021:A:N3    | 2.31                     | 0.46              |
| 53:1:1550:C:H2'   | 53:1:1551:A:C8    | 2.51                     | 0.46              |
| 57:7:26:A:H2'     | 57:7:27:G:O4'     | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:165:ALA:HB3  | 1:b:172:THR:HB   | 1.97                     | 0.46              |
| 4:e:32:LYS:HG2   | 4:e:156:THR:HG21 | 1.98                     | 0.46              |
| 7:h:80:THR:O     | 7:h:81:LEU:C     | 2.59                     | 0.46              |
| 23:x:17:ARG:HD3  | 23:x:17:ARG:HA   | 1.79                     | 0.46              |
| 27:C:16:THR:OG1  | 27:C:17:GLY:N    | 2.48                     | 0.46              |
| 41:Q:39:THR:HG22 | 41:Q:40:THR:N    | 2.25                     | 0.46              |
| 42:R:24:VAL:HG23 | 42:R:28:ARG:HB3  | 1.98                     | 0.46              |
| 43:S:42:ASN:O    | 43:S:46:LYS:HG2  | 2.15                     | 0.46              |
| 46:V:13:SER:O    | 46:V:21:VAL:HG22 | 2.16                     | 0.46              |
| 47:W:70:THR:HG23 | 47:W:72:ARG:H    | 1.80                     | 0.46              |
| 52:3:175:C:O2'   | 52:3:176:C:H5'   | 2.16                     | 0.46              |
| 52:3:784:A:H2'   | 52:3:785:G:H8    | 1.77                     | 0.46              |
| 52:3:981:U:H2'   | 52:3:982:U:C5    | 2.51                     | 0.46              |
| 53:1:818:G:O2'   | 53:1:819:A:H5''  | 2.16                     | 0.46              |
| 53:1:1590:A:H2'  | 53:1:1591:A:C8   | 2.51                     | 0.46              |
| 53:1:1736:U:H2'  | 53:1:1737:G:O4'  | 2.15                     | 0.46              |
| 53:1:1779:U:OP1  | 53:1:1780:A:H5'  | 2.16                     | 0.46              |
| 53:1:1786:A:H1'  | 53:1:1938:A:N6   | 2.30                     | 0.46              |
| 53:1:1858:A:H1'  | 53:1:1885:A:C2   | 2.51                     | 0.46              |
| 55:5:16:C:O2'    | 55:5:17:C:H5'    | 2.16                     | 0.46              |
| 16:q:65:ASN:ND2  | 53:1:1010:A:OP1  | 2.48                     | 0.46              |
| 19:t:47:VAL:HG13 | 19:t:51:PHE:HD2  | 1.79                     | 0.46              |
| 21:v:84:PRO:HD2  | 53:1:1118:C:H5'' | 1.98                     | 0.46              |
| 22:w:18:GLY:O    | 22:w:20:LYS:NZ   | 2.49                     | 0.46              |
| 24:y:19:LEU:O    | 24:y:23:ARG:HB2  | 2.16                     | 0.46              |
| 33:I:186:GLU:HB3 | 33:I:189:ASP:OD2 | 2.15                     | 0.46              |
| 35:K:75:GLU:HA   | 35:K:78:PHE:CD2  | 2.51                     | 0.46              |
| 41:Q:23:LEU:HD13 | 41:Q:29:LYS:HZ3  | 1.76                     | 0.46              |
| 46:V:29:LYS:HB2  | 46:V:36:PHE:CE1  | 2.51                     | 0.46              |
| 52:3:58:C:O2'    | 52:3:59:A:H5'    | 2.16                     | 0.46              |
| 52:3:762:U:H2'   | 52:3:763:G:H8    | 1.80                     | 0.46              |
| 52:3:1508:A:H2'  | 52:3:1509:C:C6   | 2.50                     | 0.46              |
| 53:1:184:C:H4'   | 53:1:217:A:H2    | 1.81                     | 0.46              |
| 53:1:445:C:O2'   | 53:1:446:G:H5'   | 2.15                     | 0.46              |
| 53:1:1028:A:N6   | 53:1:1125:G:H2'  | 2.31                     | 0.46              |
| 57:7:6:G:H3'     | 57:7:7:A:C5'     | 2.43                     | 0.46              |
| 58:8:14:ASN:ND2  | 58:8:272:GLY:O   | 2.48                     | 0.46              |
| 58:8:216:GLU:OE2 | 58:8:230:GLY:HA2 | 2.15                     | 0.46              |
| 2:c:105:LYS:HG3  | 2:c:106:LYS:HG3  | 1.98                     | 0.45              |
| 13:n:47:VAL:O    | 13:n:50:PRO:HD2  | 2.16                     | 0.45              |
| 19:t:9:LYS:HA    | 24:y:29:ARG:HH12 | 1.81                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:w:55:LEU:HD12 | 22:w:76:ILE:HD12  | 1.98                     | 0.45              |
| 23:x:18:SER:OG   | 23:x:19:HIS:N     | 2.50                     | 0.45              |
| 23:x:38:TRP:HB2  | 23:x:45:PHE:CE1   | 2.51                     | 0.45              |
| 25:z:5:LYS:HB2   | 25:z:57:GLU:HG2   | 1.99                     | 0.45              |
| 32:H:78:LYS:H    | 32:H:81:GLU:HG2   | 1.81                     | 0.45              |
| 32:H:107:LYS:HB3 | 32:H:143:LEU:HD21 | 1.99                     | 0.45              |
| 33:I:53:GLN:HG3  | 33:I:202:LEU:HD13 | 1.97                     | 0.45              |
| 36:L:30:MET:SD   | 36:L:35:LYS:HB2   | 2.57                     | 0.45              |
| 52:3:423:G:H2'   | 52:3:424:G:H5'    | 1.97                     | 0.45              |
| 52:3:483:C:H2'   | 52:3:484:G:C8     | 2.52                     | 0.45              |
| 52:3:912:C:O2'   | 52:3:913:A:H5'    | 2.15                     | 0.45              |
| 52:3:1251:A:H2'  | 52:3:1252:A:C8    | 2.51                     | 0.45              |
| 52:3:1323:G:H2'  | 52:3:1324:A:C8    | 2.51                     | 0.45              |
| 52:3:1342:C:H2'  | 52:3:1343:G:C8    | 2.50                     | 0.45              |
| 52:3:1502:A:C8   | 52:3:1505:G:N2    | 2.84                     | 0.45              |
| 53:1:467:G:HO2'  | 53:1:468:G:H5'    | 1.81                     | 0.45              |
| 53:1:548:G:H2'   | 53:1:549:G:O4'    | 2.16                     | 0.45              |
| 53:1:1026:G:H2'  | 53:1:1027:A:H8    | 1.81                     | 0.45              |
| 53:1:1357:C:H2'  | 53:1:1358:G:O4'   | 2.17                     | 0.45              |
| 53:1:1479:G:O2'  | 53:1:1480:C:H5'   | 2.16                     | 0.45              |
| 53:1:2432:A:H1'  | 55:6:75:C:C4'     | 2.46                     | 0.45              |
| 55:6:41:C:H2'    | 55:6:42:G:C8      | 2.51                     | 0.45              |
| 58:8:43:ALA:O    | 58:8:45:ARG:NH2   | 2.49                     | 0.45              |
| 1:b:159:THR:HG21 | 53:1:1819:A:H5''  | 1.98                     | 0.45              |
| 7:h:118:ILE:N    | 7:h:119:PRO:CD    | 2.78                     | 0.45              |
| 12:m:12:MET:HE2  | 12:m:71:LYS:NZ    | 2.31                     | 0.45              |
| 12:m:14:LYS:NZ   | 53:1:956:G:N7     | 2.63                     | 0.45              |
| 26:B:49:ARG:HG2  | 53:1:2884:U:C5    | 2.52                     | 0.45              |
| 35:K:18:VAL:CG2  | 35:K:19:PRO:HD3   | 2.46                     | 0.45              |
| 52:3:82:G:C2'    | 52:3:83:C:H5'     | 2.46                     | 0.45              |
| 52:3:1195:C:H5'' | 52:3:1196:A:OP2   | 2.16                     | 0.45              |
| 53:1:466:A:C2'   | 53:1:467:G:H5'    | 2.46                     | 0.45              |
| 53:1:718:A:H2'   | 53:1:719:C:H5'    | 1.99                     | 0.45              |
| 53:1:1430:G:H2'  | 53:1:1431:A:O4'   | 2.16                     | 0.45              |
| 53:1:2581:G:H2'  | 53:1:2581:G:N3    | 2.30                     | 0.45              |
| 53:1:2687:U:H2'  | 53:1:2688:G:O4'   | 2.16                     | 0.45              |
| 3:d:68:ALA:HA    | 53:1:1255:U:C5    | 2.51                     | 0.45              |
| 9:j:113:PRO:HB2  | 53:1:557:C:H5''   | 1.98                     | 0.45              |
| 15:p:24:THR:HG22 | 15:p:43:GLU:OE2   | 2.17                     | 0.45              |
| 15:p:63:ILE:HG23 | 15:p:63:ILE:O     | 2.16                     | 0.45              |
| 23:x:55:MET:SD   | 53:1:2091:C:H4'   | 2.57                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:G:69:VAL:HG12 | 31:G:91:VAL:HG22  | 1.98                     | 0.45              |
| 41:Q:56:LEU:HD12 | 41:Q:60:PHE:HB2   | 1.98                     | 0.45              |
| 48:X:36:ARG:HB3  | 52:3:1320:C:N4    | 2.32                     | 0.45              |
| 50:Z:50:SER:CA   | 50:Z:53:LYS:HE2   | 2.45                     | 0.45              |
| 52:3:162:A:H2'   | 52:3:163:C:H5'    | 1.98                     | 0.45              |
| 52:3:240:G:H2'   | 52:3:241:G:C8     | 2.51                     | 0.45              |
| 52:3:1463:U:H2'  | 52:3:1464:U:C6    | 2.52                     | 0.45              |
| 53:1:149:A:H2'   | 53:1:150:U:C6     | 2.51                     | 0.45              |
| 53:1:519:U:H2'   | 53:1:520:G:H8     | 1.81                     | 0.45              |
| 53:1:534:U:H2'   | 53:1:535:G:H8     | 1.81                     | 0.45              |
| 53:1:554:U:H2'   | 53:1:555:G:O4'    | 2.16                     | 0.45              |
| 53:1:1639:C:O2'  | 53:1:1640:A:H5'   | 2.16                     | 0.45              |
| 53:1:2121:G:H2'  | 53:1:2122:U:O4'   | 2.16                     | 0.45              |
| 53:1:2292:U:H2'  | 53:1:2293:G:C8    | 2.51                     | 0.45              |
| 53:1:2656:U:H2'  | 53:1:2657:A:H5'   | 1.97                     | 0.45              |
| 57:7:45:U:C3'    | 57:7:46:G:H5''    | 2.46                     | 0.45              |
| 18:s:3:THR:HG21  | 18:s:58:ALA:HB2   | 1.98                     | 0.45              |
| 33:I:67:LEU:HB3  | 52:3:546:A:OP2    | 2.16                     | 0.45              |
| 34:J:160:VAL:O   | 34:J:163:ILE:HG12 | 2.16                     | 0.45              |
| 36:L:56:SER:OG   | 36:L:59:GLU:HG2   | 2.15                     | 0.45              |
| 36:L:83:THR:HG23 | 36:L:83:THR:O     | 2.17                     | 0.45              |
| 51:a:195:ALA:O   | 51:a:198:LYS:HG3  | 2.15                     | 0.45              |
| 52:3:460:A:H2'   | 52:3:461:A:C8     | 2.52                     | 0.45              |
| 52:3:1005:A:H2'  | 52:3:1006:G:H5'   | 1.96                     | 0.45              |
| 53:1:696:G:O2'   | 53:1:697:G:H5'    | 2.16                     | 0.45              |
| 53:1:1181:U:H2'  | 53:1:1182:G:H8    | 1.80                     | 0.45              |
| 53:1:1903:G:H2'  | 53:1:1904:G:C8    | 2.52                     | 0.45              |
| 53:1:2153:C:H2'  | 53:1:2154:A:C8    | 2.52                     | 0.45              |
| 53:1:2888:C:H2'  | 53:1:2889:C:C6    | 2.50                     | 0.45              |
| 4:e:38:GLY:HA3   | 53:1:2312:U:O2    | 2.16                     | 0.45              |
| 31:G:173:LYS:O   | 31:G:177:ASN:ND2  | 2.50                     | 0.45              |
| 36:L:142:ARG:CB  | 55:6:41:C:H4'     | 2.44                     | 0.45              |
| 40:P:91:GLY:O    | 40:P:93:GLU:N     | 2.42                     | 0.45              |
| 41:Q:8:ARG:HH12  | 52:3:881:G:P      | 2.40                     | 0.45              |
| 46:V:5:ARG:NH1   | 52:3:636:U:H5'    | 2.32                     | 0.45              |
| 52:3:1296:C:H4'  | 52:3:1302:C:H41   | 1.81                     | 0.45              |
| 52:3:1368:A:O2'  | 52:3:1369:C:H5'   | 2.16                     | 0.45              |
| 52:3:1515:G:O2'  | 52:3:1516:G:H5'   | 2.17                     | 0.45              |
| 53:1:760:G:H2'   | 53:1:761:A:O4'    | 2.16                     | 0.45              |
| 53:1:822:G:H5'   | 53:1:822:G:H8     | 1.80                     | 0.45              |
| 53:1:1447:C:H2'  | 53:1:1448:G:C8    | 2.52                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:1642:G:O2'  | 53:1:1643:G:H5'   | 2.16                     | 0.45              |
| 53:1:2105:U:H2'  | 53:1:2106:U:O4'   | 2.16                     | 0.45              |
| 53:1:2106:U:H2'  | 53:1:2107:G:C8    | 2.52                     | 0.45              |
| 53:1:2263:C:H4'  | 53:1:2329:U:H4'   | 1.99                     | 0.45              |
| 53:1:2360:G:H2'  | 53:1:2361:G:H5'   | 1.97                     | 0.45              |
| 53:1:2888:C:H2'  | 53:1:2889:C:H6    | 1.82                     | 0.45              |
| 54:2:97:C:H2'    | 54:2:98:G:O4'     | 2.16                     | 0.45              |
| 58:8:20:HIS:CE1  | 58:8:21:VAL:HG12  | 2.52                     | 0.45              |
| 58:8:309:VAL:HA  | 58:8:387:GLY:HA2  | 1.99                     | 0.45              |
| 3:d:117:ARG:NH2  | 3:d:183:PHE:O     | 2.50                     | 0.45              |
| 7:h:118:ILE:CB   | 7:h:119:PRO:HD3   | 2.46                     | 0.45              |
| 14:o:49:VAL:HG22 | 14:o:85:LYS:HG3   | 1.98                     | 0.45              |
| 26:B:12:ARG:NH2  | 53:1:517:C:OP1    | 2.50                     | 0.45              |
| 32:H:4:VAL:HG22  | 32:H:5:HIS:N      | 2.31                     | 0.45              |
| 38:N:86:LEU:HD22 | 38:N:89:TYR:HD2   | 1.81                     | 0.45              |
| 40:P:87:GLY:H    | 40:P:113:THR:HG22 | 1.81                     | 0.45              |
| 47:W:27:THR:HA   | 47:W:30:ASN:ND2   | 2.32                     | 0.45              |
| 52:3:936:C:H2'   | 52:3:937:A:O4'    | 2.17                     | 0.45              |
| 52:3:1402:C:H2'  | 52:3:1403:C:O4'   | 2.16                     | 0.45              |
| 53:1:395:U:H2'   | 53:1:396:G:H8     | 1.82                     | 0.45              |
| 53:1:438:G:H2'   | 53:1:439:A:H8     | 1.82                     | 0.45              |
| 53:1:1326:U:H2'  | 53:1:1327:A:C8    | 2.52                     | 0.45              |
| 53:1:1365:A:N3   | 53:1:1365:A:H2'   | 2.30                     | 0.45              |
| 53:1:1549:A:H2'  | 53:1:1550:C:C6    | 2.52                     | 0.45              |
| 53:1:2691:C:H2'  | 53:1:2692:G:C8    | 2.51                     | 0.45              |
| 53:1:2756:U:H4'  | 53:1:2757:A:OP1   | 2.17                     | 0.45              |
| 53:1:2788:C:H2'  | 53:1:2789:C:C6    | 2.52                     | 0.45              |
| 1:b:129:LEU:N    | 1:b:129:LEU:HD23  | 2.32                     | 0.45              |
| 1:b:224:MET:HE2  | 53:1:782:A:C6     | 2.52                     | 0.45              |
| 4:e:107:VAL:O    | 4:e:110:ILE:HG12  | 2.17                     | 0.45              |
| 4:e:125:GLY:HA2  | 4:e:162:ASP:HA    | 1.99                     | 0.45              |
| 32:H:76:ILE:HD12 | 32:H:83:VAL:HG21  | 1.99                     | 0.45              |
| 35:K:76:THR:HA   | 35:K:79:ARG:NH1   | 2.32                     | 0.45              |
| 41:Q:30:ARG:HB2  | 52:3:363:A:H5'    | 1.98                     | 0.45              |
| 41:Q:100:ALA:O   | 41:Q:101:LEU:O    | 2.35                     | 0.45              |
| 43:S:68:ARG:HH12 | 52:3:1202:U:H5'   | 1.81                     | 0.45              |
| 46:V:46:HIS:CA   | 46:V:70:LYS:HD2   | 2.47                     | 0.45              |
| 52:3:279:A:H5''  | 52:3:280:C:H3'    | 1.99                     | 0.45              |
| 52:3:661:G:O2'   | 52:3:662:U:H5'    | 2.16                     | 0.45              |
| 52:3:1173:U:H2'  | 52:3:1174:G:H8    | 1.82                     | 0.45              |
| 53:1:711:G:H2'   | 53:1:712:G:O4'    | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:996:A:H2'    | 53:1:997:G:C8     | 2.52                     | 0.45              |
| 53:1:1979:U:O2'   | 53:1:1980:G:H5'   | 2.17                     | 0.45              |
| 53:1:2898:U:H2'   | 53:1:2899:A:C8    | 2.51                     | 0.45              |
| 54:2:37:C:H42     | 54:2:49:C:H1'     | 1.81                     | 0.45              |
| 4:e:120:SER:OG    | 53:1:2304:G:H5'   | 2.17                     | 0.45              |
| 5:f:66:THR:OG1    | 53:1:2748:A:H1'   | 2.17                     | 0.45              |
| 5:f:136:ASP:OD2   | 5:f:139:VAL:HG23  | 2.16                     | 0.45              |
| 6:g:48:GLU:HA     | 6:g:52:ALA:HB3    | 1.99                     | 0.45              |
| 34:J:22:LYS:HG3   | 52:3:1081:A:H5'   | 1.99                     | 0.45              |
| 36:L:36:SER:O     | 36:L:39:GLU:HG2   | 2.16                     | 0.45              |
| 38:N:70:GLY:O     | 38:N:74:GLN:HG3   | 2.16                     | 0.45              |
| 44:T:32:THR:HG22  | 44:T:36:ASN:ND2   | 2.32                     | 0.45              |
| 52:3:56:U:H2'     | 52:3:57:G:H8      | 1.81                     | 0.45              |
| 52:3:202:G:H2'    | 52:3:203:G:H8     | 1.82                     | 0.45              |
| 52:3:824:G:H2'    | 52:3:825:A:H8     | 1.82                     | 0.45              |
| 53:1:256:A:O2'    | 53:1:257:C:H5'    | 2.17                     | 0.45              |
| 53:1:779:U:H2'    | 53:1:780:G:C8     | 2.51                     | 0.45              |
| 53:1:1468:U:H2'   | 53:1:1522:A:N6    | 2.32                     | 0.45              |
| 53:1:2266:A:H4'   | 53:1:2267:A:C2    | 2.52                     | 0.45              |
| 58:8:19:GLY:H     | 58:8:119:HIS:CD2  | 2.35                     | 0.45              |
| 2:c:107:VAL:HG22  | 2:c:175:LEU:O     | 2.15                     | 0.45              |
| 4:e:122:ASP:OD1   | 4:e:126:ASN:N     | 2.50                     | 0.45              |
| 11:l:122:VAL:HG11 | 11:l:127:VAL:HG21 | 1.99                     | 0.45              |
| 18:s:15:GLN:NE2   | 53:1:1266:G:C8    | 2.84                     | 0.45              |
| 24:y:16:THR:O     | 24:y:19:LEU:HB3   | 2.16                     | 0.45              |
| 25:z:30:ARG:HD3   | 25:z:30:ARG:H     | 1.82                     | 0.45              |
| 32:H:45:GLU:HG3   | 32:H:46:LEU:HD12  | 1.98                     | 0.45              |
| 34:J:105:ILE:HG23 | 34:J:123:LEU:HA   | 1.99                     | 0.45              |
| 45:U:80:LYS:N     | 45:U:80:LYS:HD3   | 2.32                     | 0.45              |
| 49:Y:2:ASN:OD1    | 49:Y:3:ILE:N      | 2.50                     | 0.45              |
| 52:3:1011:C:H2'   | 52:3:1012:A:C8    | 2.52                     | 0.45              |
| 52:3:1033:G:C3'   | 52:3:1034:G:H5''  | 2.47                     | 0.45              |
| 53:1:940:G:H2'    | 53:1:941:A:H5''   | 1.98                     | 0.45              |
| 53:1:1028:A:H2'   | 53:1:1029:A:C8    | 2.52                     | 0.45              |
| 57:7:45:U:H3'     | 57:7:46:G:H5''    | 1.99                     | 0.45              |
| 1:b:180:MET:HB2   | 1:b:268:ARG:HB2   | 1.98                     | 0.45              |
| 1:b:230:PRO:HG2   | 1:b:245:THR:O     | 2.16                     | 0.45              |
| 10:k:106:GLU:N    | 10:k:106:GLU:OE2  | 2.49                     | 0.45              |
| 13:n:36:THR:OG1   | 13:n:37:THR:N     | 2.50                     | 0.45              |
| 16:q:48:ASP:HA    | 16:q:51:GLN:HB3   | 1.98                     | 0.45              |
| 21:v:6:ALA:CB     | 21:v:42:LEU:HB3   | 2.47                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 21:v:82:TYR:CD2  | 21:v:83:LYS:HE2   | 2.52                     | 0.45              |
| 32:H:172:VAL:O   | 32:H:172:VAL:HG13 | 2.17                     | 0.45              |
| 33:I:149:LYS:C   | 33:I:150:LYS:HG3  | 2.42                     | 0.45              |
| 39:O:32:THR:O    | 39:O:83:THR:OG1   | 2.35                     | 0.45              |
| 44:T:44:GLU:HG2  | 44:T:45:HIS:H     | 1.82                     | 0.45              |
| 53:1:394:C:O2'   | 53:1:395:U:H5'    | 2.17                     | 0.45              |
| 53:1:419:U:H2'   | 53:1:420:C:C6     | 2.52                     | 0.45              |
| 53:1:694:U:OP1   | 53:1:1569:A:H1'   | 2.16                     | 0.45              |
| 53:1:2296:U:H4'  | 53:1:2297:A:O5'   | 2.17                     | 0.45              |
| 53:1:2605:U:H2'  | 53:1:2606:C:C6    | 2.52                     | 0.45              |
| 53:1:2698:U:H2'  | 53:1:2699:C:H6    | 1.80                     | 0.45              |
| 57:7:68:C:H2'    | 57:7:69:G:C8      | 2.51                     | 0.45              |
| 1:b:251:THR:OG1  | 1:b:252:LYS:N     | 2.51                     | 0.44              |
| 7:h:123:ILE:H    | 7:h:123:ILE:CD1   | 2.24                     | 0.44              |
| 13:n:65:LEU:HD12 | 13:n:65:LEU:HA    | 1.87                     | 0.44              |
| 21:v:82:TYR:CE2  | 21:v:83:LYS:HE2   | 2.52                     | 0.44              |
| 24:y:49:ASP:HA   | 24:y:52:ARG:NH2   | 2.32                     | 0.44              |
| 32:H:14:VAL:HG23 | 32:H:15:LYS:HG2   | 1.98                     | 0.44              |
| 35:K:46:GLN:HE21 | 35:K:55:HIS:HB3   | 1.82                     | 0.44              |
| 38:N:28:VAL:HG13 | 38:N:63:TYR:HA    | 1.99                     | 0.44              |
| 52:3:501:C:H1'   | 52:3:549:C:H1'    | 1.99                     | 0.44              |
| 52:3:580:C:H2'   | 52:3:581:G:O4'    | 2.17                     | 0.44              |
| 52:3:1374:A:H2'  | 52:3:1375:A:C8    | 2.52                     | 0.44              |
| 53:1:473:G:C2'   | 53:1:474:G:H5'    | 2.47                     | 0.44              |
| 53:1:2149:U:H2'  | 53:1:2150:C:O4'   | 2.17                     | 0.44              |
| 53:1:2655:G:O2'  | 53:1:2656:U:H5    | 1.99                     | 0.44              |
| 54:2:66:A:H5''   | 54:2:67:G:OP1     | 2.17                     | 0.44              |
| 54:2:118:C:H2'   | 54:2:119:A:C8     | 2.52                     | 0.44              |
| 58:8:8:ARG:HH22  | 58:8:266:LEU:HD11 | 1.82                     | 0.44              |
| 4:e:102:LEU:HD11 | 4:e:153:ILE:HD13  | 1.98                     | 0.44              |
| 6:g:99:ILE:HG21  | 6:g:115:VAL:HG21  | 1.99                     | 0.44              |
| 10:k:9:ASN:O     | 10:k:83:ALA:HA    | 2.17                     | 0.44              |
| 16:q:50:ARG:HG3  | 16:q:50:ARG:NH1   | 2.32                     | 0.44              |
| 27:C:12:SER:HB3  | 27:C:48:TYR:CE1   | 2.52                     | 0.44              |
| 32:H:2:GLN:NE2   | 32:H:3:LYS:HG3    | 2.33                     | 0.44              |
| 38:N:34:LEU:HD23 | 38:N:34:LEU:C     | 2.42                     | 0.44              |
| 42:R:6:ILE:O     | 42:R:7:ASN:C      | 2.59                     | 0.44              |
| 46:V:45:VAL:HG21 | 46:V:60:ILE:HG21  | 1.99                     | 0.44              |
| 50:Z:6:ARG:O     | 50:Z:7:GLU:C      | 2.60                     | 0.44              |
| 52:3:419:C:O2'   | 52:3:420:U:H5'    | 2.18                     | 0.44              |
| 52:3:710:G:H2'   | 52:3:711:G:H8     | 1.83                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:3:855:U:H2'    | 52:3:856:C:C6     | 2.52                     | 0.44              |
| 52:3:1038:C:H2'   | 52:3:1039:G:C8    | 2.53                     | 0.44              |
| 52:3:1201:A:C1'   | 52:3:1202:U:OP2   | 2.63                     | 0.44              |
| 53:1:161:A:H3'    | 53:1:162:U:H5''   | 1.98                     | 0.44              |
| 53:1:1060:U:H4'   | 53:1:1061:U:O5'   | 2.17                     | 0.44              |
| 53:1:2246:G:H2'   | 53:1:2247:A:C8    | 2.52                     | 0.44              |
| 53:1:2743:U:C2'   | 53:1:2744:G:H5''  | 2.46                     | 0.44              |
| 57:7:25:C:H2'     | 57:7:26:A:C4'     | 2.47                     | 0.44              |
| 58:8:56:GLU:CG    | 58:8:63:ILE:HG12  | 2.47                     | 0.44              |
| 1:b:249:VAL:HG13  | 1:b:249:VAL:O     | 2.17                     | 0.44              |
| 5:f:16:VAL:HG22   | 5:f:25:ILE:HG12   | 1.99                     | 0.44              |
| 12:m:12:MET:HA    | 53:1:910:A:N6     | 2.19                     | 0.44              |
| 17:r:24:LYS:HA    | 17:r:94:THR:OG1   | 2.17                     | 0.44              |
| 31:G:96:LEU:H     | 31:G:99:MET:HE2   | 1.81                     | 0.44              |
| 31:G:213:LEU:HA   | 31:G:216:VAL:HB   | 1.99                     | 0.44              |
| 32:H:149:LYS:HE2  | 32:H:166:TRP:HE3  | 1.82                     | 0.44              |
| 33:I:131:ILE:HG21 | 52:3:620:C:O2     | 2.17                     | 0.44              |
| 40:P:12:ARG:NH1   | 40:P:76:TYR:OH    | 2.51                     | 0.44              |
| 52:3:195:A:H2'    | 52:3:196:A:C8     | 2.52                     | 0.44              |
| 52:3:556:C:O2'    | 52:3:557:G:H5'    | 2.17                     | 0.44              |
| 52:3:665:A:O4'    | 52:3:733:G:H1'    | 2.17                     | 0.44              |
| 53:1:1947:C:H2'   | 53:1:1948:G:H8    | 1.82                     | 0.44              |
| 53:1:2285:C:H5'   | 53:1:2288:A:N6    | 2.32                     | 0.44              |
| 2:c:48:ILE:HG23   | 2:c:84:LEU:HD21   | 2.00                     | 0.44              |
| 5:f:102:ILE:HD11  | 5:f:116:LEU:HD11  | 1.98                     | 0.44              |
| 11:l:13:LYS:HE3   | 53:1:1245:G:OP1   | 2.17                     | 0.44              |
| 12:m:56:ALA:HB2   | 12:m:119:LEU:HD12 | 1.99                     | 0.44              |
| 16:q:73:ILE:HD11  | 16:q:77:LYS:HB3   | 2.00                     | 0.44              |
| 19:t:80:TRP:HZ3   | 19:t:82:LYS:HB3   | 1.81                     | 0.44              |
| 25:z:45:GLY:HA3   | 53:1:852:U:H5'    | 1.99                     | 0.44              |
| 29:E:4:LYS:HE2    | 53:1:253:C:OP2    | 2.17                     | 0.44              |
| 41:Q:20:VAL:HB    | 41:Q:94:TYR:HE1   | 1.82                     | 0.44              |
| 41:Q:23:LEU:HD13  | 41:Q:29:LYS:HZ1   | 1.81                     | 0.44              |
| 48:X:35:ARG:O     | 48:X:71:GLY:N     | 2.51                     | 0.44              |
| 49:Y:26:MET:O     | 49:Y:29:THR:HG22  | 2.17                     | 0.44              |
| 51:a:52:ALA:HB3   | 51:a:53:ARG:NH1   | 2.33                     | 0.44              |
| 51:a:184:LYS:HA   | 51:a:184:LYS:HD3  | 1.85                     | 0.44              |
| 52:3:1352:C:H2'   | 52:3:1353:G:H8    | 1.80                     | 0.44              |
| 53:1:158:U:H2'    | 53:1:159:G:O4'    | 2.17                     | 0.44              |
| 53:1:1469:A:H2'   | 53:1:1470:A:C8    | 2.53                     | 0.44              |
| 53:1:2292:U:H2'   | 53:1:2293:G:H8    | 1.81                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:2467:C:H2'  | 53:1:2468:A:O4'   | 2.17                     | 0.44              |
| 55:5:47:U:H3'    | 55:5:48:C:H5'     | 2.00                     | 0.44              |
| 55:6:34:C:O2     | 55:6:34:C:H3'     | 2.18                     | 0.44              |
| 2:c:16:THR:OG1   | 2:c:18:ASP:OD1    | 2.35                     | 0.44              |
| 5:f:175:LYS:HD3  | 5:f:175:LYS:HA    | 1.80                     | 0.44              |
| 10:k:69:VAL:HG22 | 10:k:70:ARG:N     | 2.32                     | 0.44              |
| 12:m:64:TRP:HE1  | 53:1:873:C:H4'    | 1.83                     | 0.44              |
| 31:G:49:PHE:CD1  | 31:G:199:ILE:HD13 | 2.53                     | 0.44              |
| 32:H:76:ILE:HG23 | 32:H:77:GLY:N     | 2.32                     | 0.44              |
| 35:K:98:GLU:HB3  | 35:K:99:ALA:H     | 1.66                     | 0.44              |
| 39:O:17:LEU:O    | 39:O:20:GLN:NE2   | 2.51                     | 0.44              |
| 39:O:59:LYS:HD3  | 52:3:972:C:O3'    | 2.17                     | 0.44              |
| 43:S:50:LEU:HD12 | 43:S:51:PRO:CD    | 2.40                     | 0.44              |
| 46:V:56:ASP:N    | 46:V:56:ASP:OD1   | 2.50                     | 0.44              |
| 48:X:28:LYS:HG2  | 48:X:29:PRO:HD2   | 2.00                     | 0.44              |
| 52:3:1061:G:H2'  | 52:3:1062:U:O4'   | 2.18                     | 0.44              |
| 52:3:1138:G:H3'  | 52:3:1138:G:N3    | 2.32                     | 0.44              |
| 53:1:503:A:H5''  | 53:1:505:A:OP1    | 2.18                     | 0.44              |
| 53:1:783:A:H2'   | 53:1:784:G:H5'    | 1.99                     | 0.44              |
| 53:1:2277:G:C2'  | 53:1:2278:A:H5''  | 2.46                     | 0.44              |
| 53:1:2427:C:C5'  | 53:1:2429:G:H5'   | 2.45                     | 0.44              |
| 2:c:123:LYS:NZ   | 53:1:2724:U:H5''  | 2.32                     | 0.44              |
| 3:d:77:ILE:HG13  | 3:d:78:TRP:HD1    | 1.83                     | 0.44              |
| 8:i:89:SER:N     | 53:1:1063:G:O2'   | 2.51                     | 0.44              |
| 16:q:90:ASP:OD2  | 53:1:996:A:H4'    | 2.18                     | 0.44              |
| 17:r:33:VAL:HG22 | 17:r:34:GLU:H     | 1.82                     | 0.44              |
| 17:r:33:VAL:HG22 | 17:r:34:GLU:N     | 2.32                     | 0.44              |
| 18:s:15:GLN:O    | 18:s:19:LEU:HD12  | 2.17                     | 0.44              |
| 27:C:25:ASN:HD22 | 53:1:2285:C:P     | 2.41                     | 0.44              |
| 31:G:141:GLU:HA  | 31:G:144:GLU:HB3  | 2.00                     | 0.44              |
| 34:J:100:GLU:H   | 34:J:121:ASN:HD22 | 1.66                     | 0.44              |
| 35:K:51:ILE:O    | 35:K:52:ASN:HB2   | 2.17                     | 0.44              |
| 37:M:55:LYS:HD3  | 52:3:652:U:O2'    | 2.17                     | 0.44              |
| 43:S:5:MET:O     | 43:S:9:GLU:HG2    | 2.18                     | 0.44              |
| 43:S:72:PHE:CZ   | 43:S:77:GLY:HA2   | 2.53                     | 0.44              |
| 45:U:21:VAL:HG23 | 45:U:21:VAL:O     | 2.18                     | 0.44              |
| 46:V:48:GLU:HB3  | 46:V:51:GLU:OE1   | 2.18                     | 0.44              |
| 51:a:4:LEU:HD22  | 51:a:8:MET:HB3    | 2.00                     | 0.44              |
| 52:3:367:U:C5'   | 58:8:280:ARG:HH21 | 2.30                     | 0.44              |
| 53:1:368:A:C2'   | 53:1:369:U:H5'    | 2.47                     | 0.44              |
| 53:1:700:G:O2'   | 53:1:701:G:H5'    | 2.16                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:717:C:H2'   | 53:1:718:A:H5'    | 1.98                     | 0.44              |
| 53:1:1572:A:H2'  | 53:1:1573:G:C8    | 2.53                     | 0.44              |
| 53:1:2329:U:H2'  | 53:1:2330:G:H8    | 1.83                     | 0.44              |
| 53:1:2350:C:H2'  | 53:1:2351:G:O4'   | 2.17                     | 0.44              |
| 53:1:2628:C:H3'  | 53:1:2629:U:H5'   | 1.99                     | 0.44              |
| 58:8:143:ASP:HB3 | 58:8:146:LEU:HG   | 2.00                     | 0.44              |
| 27:C:35:LEU:HD23 | 27:C:37:LYS:HE2   | 1.99                     | 0.44              |
| 30:F:33:HIS:O    | 30:F:35:GLN:HG2   | 2.17                     | 0.44              |
| 32:H:59:PRO:HB3  | 39:O:94:ALA:HB2   | 2.00                     | 0.44              |
| 43:S:40:ARG:NH2  | 48:X:6:LYS:HG3    | 2.33                     | 0.44              |
| 52:3:113:G:H2'   | 52:3:114:U:C6     | 2.53                     | 0.44              |
| 52:3:741:G:H2'   | 52:3:742:G:C8     | 2.53                     | 0.44              |
| 52:3:834:U:H2'   | 52:3:835:U:C6     | 2.52                     | 0.44              |
| 52:3:1187:G:H2'  | 52:3:1188:A:C8    | 2.52                     | 0.44              |
| 53:1:255:A:H2'   | 53:1:256:A:C8     | 2.53                     | 0.44              |
| 53:1:275:C:H2'   | 53:1:276:U:C4'    | 2.45                     | 0.44              |
| 53:1:441:U:H2'   | 53:1:442:G:C8     | 2.53                     | 0.44              |
| 53:1:519:U:H2'   | 53:1:520:G:C8     | 2.52                     | 0.44              |
| 53:1:551:G:O2'   | 53:1:552:U:H5'    | 2.18                     | 0.44              |
| 54:2:30:C:C2'    | 54:2:31:C:H5'     | 2.48                     | 0.44              |
| 57:7:25:C:H2'    | 57:7:26:A:H4'     | 2.00                     | 0.44              |
| 58:8:123:GLY:HA2 | 58:8:126:VAL:HG12 | 2.00                     | 0.44              |
| 1:b:29:PHE:HD2   | 1:b:32:LEU:HG     | 1.82                     | 0.44              |
| 7:h:122:GLN:HB3  | 7:h:123:ILE:H     | 1.61                     | 0.44              |
| 24:y:27:ASN:O    | 24:y:31:GLN:HB2   | 2.18                     | 0.44              |
| 32:H:4:VAL:HB    | 52:3:1190:G:OP2   | 2.17                     | 0.44              |
| 33:I:140:ASP:OD1 | 33:I:181:PHE:HB3  | 2.17                     | 0.44              |
| 37:M:44:PHE:C    | 37:M:45:ILE:HD12  | 2.43                     | 0.44              |
| 39:O:40:ILE:CD1  | 52:3:1124:G:H4'   | 2.48                     | 0.44              |
| 49:Y:33:LYS:NZ   | 49:Y:52:GLU:OE1   | 2.47                     | 0.44              |
| 50:Z:36:PHE:C    | 50:Z:38:GLU:N     | 2.74                     | 0.44              |
| 52:3:67:C:H2'    | 52:3:68:G:C8      | 2.53                     | 0.44              |
| 52:3:205:A:H2'   | 52:3:206:C:O4'    | 2.18                     | 0.44              |
| 52:3:1293:C:H2'  | 52:3:1294:G:H8    | 1.83                     | 0.44              |
| 53:1:394:C:H2'   | 53:1:395:U:O4'    | 2.18                     | 0.44              |
| 53:1:970:U:H2'   | 53:1:971:G:H8     | 1.82                     | 0.44              |
| 53:1:2291:U:H2'  | 53:1:2292:U:C6    | 2.53                     | 0.44              |
| 53:1:2636:C:H2'  | 53:1:2637:U:H6    | 1.81                     | 0.44              |
| 53:1:2704:C:H2'  | 53:1:2705:A:O4'   | 2.17                     | 0.44              |
| 54:2:60:C:H2'    | 54:2:61:G:H8      | 1.81                     | 0.44              |
| 1:b:52:HIS:CD2   | 53:1:1824:G:OP2   | 2.71                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:b:156:SER:O     | 1:b:194:VAL:HG21  | 2.18                     | 0.44              |
| 10:k:86:LEU:H     | 10:k:86:LEU:HD12  | 1.83                     | 0.44              |
| 14:o:26:LEU:HD12  | 14:o:38:GLN:O     | 2.18                     | 0.44              |
| 14:o:100:HIS:HD2  | 54:2:48:U:H4'     | 1.82                     | 0.44              |
| 15:p:24:THR:OG1   | 15:p:87:ARG:NH1   | 2.51                     | 0.44              |
| 18:s:39:THR:HG23  | 18:s:39:THR:O     | 2.17                     | 0.44              |
| 19:t:72:GLN:OE1   | 19:t:72:GLN:N     | 2.50                     | 0.44              |
| 31:G:212:TYR:O    | 31:G:216:VAL:HG23 | 2.18                     | 0.44              |
| 32:H:160:GLU:CD   | 32:H:161:ILE:HG23 | 2.43                     | 0.44              |
| 34:J:129:SER:HB2  | 52:3:20:U:OP2     | 2.17                     | 0.44              |
| 36:L:115:MET:SD   | 36:L:118:ARG:NH2  | 2.90                     | 0.44              |
| 38:N:49:GLN:N     | 38:N:50:PRO:HD2   | 2.32                     | 0.44              |
| 39:O:28:THR:HA    | 39:O:31:ARG:HE    | 1.82                     | 0.44              |
| 49:Y:67:HIS:HB3   | 52:3:262:A:H5'    | 1.99                     | 0.44              |
| 50:Z:44:ARG:NH1   | 52:3:722:G:OP2    | 2.51                     | 0.44              |
| 50:Z:54:ARG:O     | 50:Z:57:LYS:HG3   | 2.18                     | 0.44              |
| 52:3:1193:G:O2'   | 52:3:1194:U:H5'   | 2.18                     | 0.44              |
| 52:3:1484:C:H2'   | 52:3:1485:U:C6    | 2.53                     | 0.44              |
| 53:1:182:A:O2'    | 53:1:183:C:H5'    | 2.18                     | 0.44              |
| 53:1:259:G:H2'    | 53:1:260:G:H8     | 1.83                     | 0.44              |
| 53:1:889:C:H2'    | 53:1:890:C:O4'    | 2.17                     | 0.44              |
| 58:8:249:LYS:HG3  | 58:8:250:GLU:H    | 1.83                     | 0.44              |
| 6:g:83:LYS:HD3    | 6:g:84:ALA:H      | 1.83                     | 0.43              |
| 13:n:29:VAL:O     | 13:n:78:LYS:HG2   | 2.18                     | 0.43              |
| 15:p:87:ARG:NH2   | 15:p:111:GLU:OE2  | 2.51                     | 0.43              |
| 30:F:11:CYS:HB3   | 30:F:33:HIS:CE1   | 2.53                     | 0.43              |
| 33:I:97:LEU:HG    | 33:I:134:TYR:HD2  | 1.82                     | 0.43              |
| 33:I:205:LYS:HB3  | 52:3:8:A:C5       | 2.52                     | 0.43              |
| 44:T:9:LYS:O      | 44:T:13:GLU:HG2   | 2.17                     | 0.43              |
| 48:X:79:TYR:CE1   | 48:X:80:ARG:HG3   | 2.53                     | 0.43              |
| 52:3:256:U:H2'    | 52:3:257:G:C8     | 2.53                     | 0.43              |
| 52:3:401:C:H2'    | 52:3:402:G:C8     | 2.53                     | 0.43              |
| 52:3:762:U:H2'    | 52:3:763:G:C8     | 2.53                     | 0.43              |
| 52:3:987:G:H2'    | 52:3:988:G:H8     | 1.83                     | 0.43              |
| 53:1:171:U:H2'    | 53:1:172:A:H8     | 1.83                     | 0.43              |
| 53:1:1601:G:C2'   | 53:1:1602:U:H5'   | 2.47                     | 0.43              |
| 53:1:2656:U:C2'   | 53:1:2657:A:H5'   | 2.48                     | 0.43              |
| 53:1:2743:U:H2'   | 53:1:2744:G:C4'   | 2.48                     | 0.43              |
| 53:1:2809:A:H2'   | 53:1:2810:A:C8    | 2.53                     | 0.43              |
| 58:8:309:VAL:HG22 | 58:8:310:TYR:N    | 2.33                     | 0.43              |
| 4:e:87:LYS:HE2    | 4:e:89:THR:HG23   | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:e:130:GLY:HA3  | 53:1:2305:U:H5'  | 2.00                     | 0.43              |
| 7:h:29:ASP:H     | 7:h:56:ARG:HH22  | 1.66                     | 0.43              |
| 8:i:54:ILE:HD11  | 8:i:71:LYS:O     | 2.19                     | 0.43              |
| 11:l:118:THR:HA  | 11:l:119:PRO:HD3 | 1.86                     | 0.43              |
| 16:q:5:ARG:H     | 16:q:5:ARG:HG2   | 1.64                     | 0.43              |
| 20:u:3:LYS:C     | 20:u:4:ILE:HD12  | 2.42                     | 0.43              |
| 31:G:66:ILE:N    | 31:G:66:ILE:HD12 | 2.32                     | 0.43              |
| 34:J:9:GLU:OE1   | 34:J:9:GLU:N     | 2.51                     | 0.43              |
| 38:N:18:VAL:HG11 | 38:N:82:ILE:HD13 | 2.00                     | 0.43              |
| 48:X:30:LEU:HB2  | 48:X:48:ILE:HD12 | 1.99                     | 0.43              |
| 49:Y:79:THR:O    | 49:Y:82:ILE:HG12 | 2.18                     | 0.43              |
| 50:Z:5:VAL:HG22  | 50:Z:19:LYS:HZ3  | 1.83                     | 0.43              |
| 52:3:423:G:C2'   | 52:3:424:G:H5'   | 2.48                     | 0.43              |
| 52:3:763:G:H2'   | 52:3:764:C:H6    | 1.83                     | 0.43              |
| 53:1:2:G:H1      | 53:1:2901:C:H42  | 1.67                     | 0.43              |
| 53:1:660:C:H2'   | 53:1:661:A:C8    | 2.53                     | 0.43              |
| 53:1:854:C:O2'   | 53:1:855:G:H5'   | 2.18                     | 0.43              |
| 53:1:1826:G:H2'  | 53:1:1827:U:C6   | 2.53                     | 0.43              |
| 53:1:1848:A:H2'  | 53:1:1849:G:O4'  | 2.18                     | 0.43              |
| 53:1:1908:C:H2'  | 53:1:1909:C:C6   | 2.53                     | 0.43              |
| 53:1:1947:C:H2'  | 53:1:1948:G:C8   | 2.53                     | 0.43              |
| 53:1:2019:A:H2   | 53:1:2035:G:H22  | 1.64                     | 0.43              |
| 53:1:2246:G:H2'  | 53:1:2247:A:H8   | 1.83                     | 0.43              |
| 54:2:66:A:H4'    | 54:2:67:G:C8     | 2.53                     | 0.43              |
| 4:e:32:LYS:HA    | 4:e:95:MET:SD    | 2.59                     | 0.43              |
| 4:e:102:LEU:O    | 4:e:106:ALA:HB3  | 2.18                     | 0.43              |
| 5:f:46:ASP:OD1   | 5:f:47:ASN:N     | 2.52                     | 0.43              |
| 11:l:10:GLU:OE1  | 11:l:10:GLU:N    | 2.50                     | 0.43              |
| 17:r:49:ILE:HG22 | 17:r:54:VAL:H    | 1.83                     | 0.43              |
| 25:z:37:ARG:HH21 | 53:1:929:U:H4'   | 1.83                     | 0.43              |
| 25:z:50:VAL:O    | 25:z:54:VAL:HG22 | 2.18                     | 0.43              |
| 43:S:21:ALA:HB2  | 52:3:1257:A:C2   | 2.54                     | 0.43              |
| 52:3:621:A:H2'   | 52:3:622:A:H8    | 1.83                     | 0.43              |
| 53:1:977:G:H4'   | 53:1:1155:A:H5'  | 2.00                     | 0.43              |
| 53:1:1287:A:C2   | 53:1:1649:G:H4'  | 2.53                     | 0.43              |
| 53:1:1427:A:H4'  | 53:1:1428:C:O4'  | 2.19                     | 0.43              |
| 53:1:1625:C:H2'  | 53:1:1626:A:O4'  | 2.19                     | 0.43              |
| 53:1:1979:U:C2'  | 53:1:1980:G:H5'  | 2.49                     | 0.43              |
| 53:1:2103:C:H2'  | 53:1:2104:C:C6   | 2.53                     | 0.43              |
| 53:1:2195:U:O2'  | 53:1:2196:C:H5'  | 2.19                     | 0.43              |
| 53:1:2432:A:H1'  | 55:6:75:C:C5'    | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:1:2457:U:O2'   | 53:1:2458:G:H5'   | 2.18                     | 0.43              |
| 53:1:2833:U:O2'   | 53:1:2834:G:H5'   | 2.18                     | 0.43              |
| 54:2:65:U:H3'     | 54:2:108:A:N6     | 2.34                     | 0.43              |
| 58:8:308:GLU:HA   | 58:8:358:LYS:HA   | 2.00                     | 0.43              |
| 1:b:226:PRO:HD3   | 1:b:233:GLY:CA    | 2.49                     | 0.43              |
| 6:g:33:GLN:HB3    | 6:g:35:LYS:HE2    | 2.00                     | 0.43              |
| 8:i:21:PRO:CB     | 8:i:22:PRO:HD3    | 2.43                     | 0.43              |
| 11:l:93:ASN:O     | 11:l:94:THR:OG1   | 2.27                     | 0.43              |
| 15:p:38:ARG:HH11  | 52:3:345:C:C5'    | 2.32                     | 0.43              |
| 16:q:92:LYS:NZ    | 53:1:995:C:O2'    | 2.47                     | 0.43              |
| 31:G:96:LEU:N     | 31:G:99:MET:HE2   | 2.33                     | 0.43              |
| 33:I:102:TYR:O    | 33:I:164:ARG:NH1  | 2.51                     | 0.43              |
| 39:O:7:ARG:HD3    | 39:O:75:ASP:OD1   | 2.18                     | 0.43              |
| 40:P:43:TRP:CZ2   | 52:3:686:U:H1'    | 2.52                     | 0.43              |
| 43:S:82:LYS:O     | 43:S:85:GLU:HG3   | 2.19                     | 0.43              |
| 46:V:42:LYS:O     | 46:V:43:LEU:HD12  | 2.18                     | 0.43              |
| 51:a:174:THR:HG22 | 51:a:176:GLY:H    | 1.83                     | 0.43              |
| 52:3:77:A:H2'     | 52:3:78:A:H8      | 1.83                     | 0.43              |
| 52:3:422:C:H4'    | 52:3:423:G:H5''   | 2.01                     | 0.43              |
| 53:1:864:G:O2'    | 53:1:865:C:H5'    | 2.18                     | 0.43              |
| 53:1:948:C:H2'    | 53:1:949:G:C8     | 2.54                     | 0.43              |
| 53:1:1704:C:H2'   | 53:1:1705:A:C8    | 2.53                     | 0.43              |
| 53:1:2194:U:H2'   | 53:1:2195:U:C6    | 2.54                     | 0.43              |
| 53:1:2743:U:H2'   | 53:1:2744:G:C5'   | 2.48                     | 0.43              |
| 53:1:2841:C:H2'   | 53:1:2842:G:H8    | 1.82                     | 0.43              |
| 58:8:153:GLU:HA   | 58:8:156:GLU:HG3  | 2.00                     | 0.43              |
| 58:8:209:LYS:HB2  | 58:8:234:ARG:HB2  | 2.00                     | 0.43              |
| 2:c:47:ALA:HA     | 2:c:84:LEU:HG     | 2.01                     | 0.43              |
| 2:c:109:VAL:HG11  | 2:c:193:VAL:HG12  | 2.01                     | 0.43              |
| 13:n:9:GLN:C      | 13:n:10:LEU:HD12  | 2.43                     | 0.43              |
| 17:r:54:VAL:HG12  | 17:r:55:ASP:OD1   | 2.18                     | 0.43              |
| 36:L:92:PRO:HA    | 36:L:95:ARG:HB2   | 2.00                     | 0.43              |
| 37:M:50:VAL:HG22  | 37:M:50:VAL:O     | 2.18                     | 0.43              |
| 39:O:76:ILE:N     | 39:O:76:ILE:HD12  | 2.33                     | 0.43              |
| 48:X:9:PHE:CG     | 52:3:1318:A:H4'   | 2.54                     | 0.43              |
| 48:X:57:VAL:HA    | 48:X:58:PRO:HD3   | 1.73                     | 0.43              |
| 51:a:64:VAL:HG13  | 51:a:160:GLN:HE21 | 1.82                     | 0.43              |
| 52:3:626:G:H2'    | 52:3:627:G:C8     | 2.54                     | 0.43              |
| 52:3:1081:A:H2'   | 52:3:1082:A:C8    | 2.53                     | 0.43              |
| 53:1:558:U:H2'    | 53:1:559:G:C8     | 2.53                     | 0.43              |
| 53:1:2190:G:H2'   | 53:1:2191:A:H8    | 1.84                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:1:2740:A:H2'  | 53:1:2741:A:C8   | 2.54                     | 0.43              |
| 16:q:90:ASP:OD1  | 16:q:90:ASP:N    | 2.46                     | 0.43              |
| 35:K:20:GLY:O    | 35:K:24:ARG:HG3  | 2.18                     | 0.43              |
| 35:K:78:PHE:HA   | 35:K:84:VAL:HG21 | 2.01                     | 0.43              |
| 49:Y:17:ARG:O    | 49:Y:17:ARG:HD2  | 2.19                     | 0.43              |
| 50:Z:50:SER:HA   | 50:Z:53:LYS:HG2  | 2.00                     | 0.43              |
| 52:3:421:U:O2'   | 52:3:422:C:P     | 2.77                     | 0.43              |
| 52:3:552:U:H2'   | 52:3:553:A:C8    | 2.53                     | 0.43              |
| 52:3:1230:C:H2'  | 52:3:1231:G:H8   | 1.83                     | 0.43              |
| 53:1:804:A:H2'   | 53:1:806:C:C4    | 2.54                     | 0.43              |
| 53:1:1029:A:H2'  | 53:1:1030:C:O4'  | 2.18                     | 0.43              |
| 53:1:1091:G:O2'  | 53:1:1092:C:H5'  | 2.19                     | 0.43              |
| 53:1:2187:U:H2'  | 53:1:2188:U:C6   | 2.54                     | 0.43              |
| 53:1:2366:A:H2'  | 53:1:2367:G:O4'  | 2.19                     | 0.43              |
| 53:1:2545:G:H2'  | 53:1:2546:U:H5'  | 2.00                     | 0.43              |
| 2:c:208:LYS:HG2  | 53:1:2733:A:N1   | 2.33                     | 0.43              |
| 4:e:115:GLY:C    | 4:e:116:LEU:HD12 | 2.43                     | 0.43              |
| 20:u:17:ASP:HA   | 20:u:20:LYS:HE2  | 1.99                     | 0.43              |
| 31:G:69:VAL:HG22 | 31:G:161:PHE:O   | 2.19                     | 0.43              |
| 36:L:75:LYS:HE3  | 36:L:75:LYS:HB2  | 1.82                     | 0.43              |
| 42:R:3:ILE:O     | 42:R:5:GLY:N     | 2.48                     | 0.43              |
| 47:W:70:THR:HG22 | 47:W:73:HIS:CD2  | 2.53                     | 0.43              |
| 50:Z:28:LEU:HD12 | 50:Z:28:LEU:HA   | 1.85                     | 0.43              |
| 52:3:212:G:H2'   | 52:3:213:G:H8    | 1.83                     | 0.43              |
| 52:3:337:G:H2'   | 52:3:338:A:H8    | 1.82                     | 0.43              |
| 52:3:741:G:H2'   | 52:3:742:G:H8    | 1.83                     | 0.43              |
| 53:1:660:C:H2'   | 53:1:661:A:H8    | 1.81                     | 0.43              |
| 53:1:2112:G:H1'  | 55:6:19:G:O2'    | 2.18                     | 0.43              |
| 55:6:21:A:N1     | 55:6:48:C:H1'    | 2.33                     | 0.43              |
| 3:d:168:ASP:CG   | 3:d:170:ARG:HE   | 2.25                     | 0.43              |
| 8:i:12:VAL:O     | 8:i:13:ALA:C     | 2.62                     | 0.43              |
| 13:n:2:ARG:NH1   | 53:1:2822:G:O6   | 2.51                     | 0.43              |
| 16:q:80:ASN:O    | 16:q:84:LYS:HG2  | 2.18                     | 0.43              |
| 34:J:152:VAL:HA  | 34:J:155:LYS:HG2 | 2.01                     | 0.43              |
| 42:R:15:VAL:HG11 | 42:R:40:GLU:HG3  | 2.01                     | 0.43              |
| 47:W:12:PHE:CG   | 47:W:13:THR:N    | 2.86                     | 0.43              |
| 52:3:56:U:H2'    | 52:3:57:G:C8     | 2.54                     | 0.43              |
| 52:3:257:G:H2'   | 52:3:258:G:H8    | 1.84                     | 0.43              |
| 52:3:526:C:H3'   | 52:3:527:G:H5''  | 2.00                     | 0.43              |
| 53:1:196:A:N3    | 53:1:196:A:H2'   | 2.33                     | 0.43              |
| 53:1:1183:U:H2'  | 53:1:1184:U:C6   | 2.54                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:1916:A:H2'  | 53:1:1917:U:O4'   | 2.19                     | 0.43              |
| 53:1:2693:G:O2'  | 53:1:2694:G:H5'   | 2.19                     | 0.43              |
| 53:1:2869:G:H2'  | 53:1:2870:C:C6    | 2.53                     | 0.43              |
| 3:d:63:LYS:HD2   | 53:1:2444:G:OP2   | 2.19                     | 0.43              |
| 3:d:131:THR:HG23 | 53:1:321:U:H5''   | 2.01                     | 0.43              |
| 5:f:116:LEU:HA   | 5:f:117:PRO:HD3   | 1.88                     | 0.43              |
| 19:t:75:GLY:HA3  | 53:1:64:A:O2'     | 2.19                     | 0.43              |
| 20:u:3:LYS:O     | 20:u:93:ARG:NH2   | 2.52                     | 0.43              |
| 32:H:67:ILE:HD12 | 32:H:67:ILE:N     | 2.34                     | 0.43              |
| 33:I:82:LYS:NZ   | 52:3:5:U:H5       | 2.15                     | 0.43              |
| 47:W:31:TYR:CD2  | 47:W:54:LEU:HD11  | 2.54                     | 0.43              |
| 52:3:41:G:H2'    | 52:3:42:G:C8      | 2.53                     | 0.43              |
| 52:3:502:A:O2'   | 52:3:503:C:H5'    | 2.19                     | 0.43              |
| 53:1:286:U:H2'   | 53:1:287:G:C8     | 2.54                     | 0.43              |
| 53:1:1506:U:H2'  | 53:1:1507:C:C6    | 2.54                     | 0.43              |
| 53:1:1799:G:H4'  | 53:1:1800:C:H6    | 1.83                     | 0.43              |
| 54:2:88:C:C4'    | 54:2:89:U:OP1     | 2.67                     | 0.43              |
| 58:8:378:ARG:HG2 | 58:8:383:THR:HA   | 1.99                     | 0.43              |
| 1:b:36:ASN:HB2   | 1:b:61:TYR:HB2    | 2.00                     | 0.43              |
| 9:j:4:PHE:O      | 16:q:63:ARG:NH2   | 2.47                     | 0.43              |
| 15:p:77:SER:O    | 15:p:80:VAL:HG12  | 2.19                     | 0.43              |
| 16:q:93:ILE:O    | 16:q:97:ILE:HG13  | 2.19                     | 0.43              |
| 30:F:2:LYS:HB2   | 30:F:35:GLN:HB3   | 2.01                     | 0.43              |
| 31:G:3:VAL:HG23  | 31:G:8:MET:HE2    | 2.01                     | 0.43              |
| 38:N:28:VAL:HG13 | 38:N:63:TYR:HD1   | 1.84                     | 0.43              |
| 40:P:63:GLN:HG3  | 40:P:98:ALA:HB2   | 2.00                     | 0.43              |
| 46:V:45:VAL:HG22 | 46:V:72:TRP:HB2   | 2.01                     | 0.43              |
| 50:Z:61:ARG:H    | 50:Z:61:ARG:HD3   | 1.83                     | 0.43              |
| 51:a:63:THR:HG21 | 51:a:192:LEU:HD12 | 2.01                     | 0.43              |
| 52:3:21:G:H2'    | 52:3:22:G:C8      | 2.53                     | 0.43              |
| 52:3:710:G:H2'   | 52:3:711:G:C8     | 2.53                     | 0.43              |
| 52:3:1353:G:O2'  | 52:3:1354:U:H5'   | 2.19                     | 0.43              |
| 52:3:1481:U:H2'  | 52:3:1482:G:C8    | 2.54                     | 0.43              |
| 53:1:11:C:H3'    | 53:1:12:U:C5'     | 2.49                     | 0.43              |
| 53:1:45:G:H5''   | 53:1:46:G:C4'     | 2.48                     | 0.43              |
| 53:1:184:C:H4'   | 53:1:217:A:C2     | 2.54                     | 0.43              |
| 53:1:464:U:H2'   | 53:1:465:G:O4'    | 2.19                     | 0.43              |
| 53:1:1199:U:H2'  | 53:1:1200:C:C6    | 2.54                     | 0.43              |
| 53:1:1259:G:H2'  | 53:1:1260:A:C8    | 2.54                     | 0.43              |
| 53:1:1903:G:H2'  | 53:1:1904:G:H8    | 1.84                     | 0.43              |
| 53:1:2345:G:H5'  | 53:1:2347:C:O4'   | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 58:8:138:CYS:HA  | 58:8:141:VAL:CG1 | 2.49                     | 0.43              |
| 4:e:32:LYS:O     | 4:e:156:THR:HG22 | 2.19                     | 0.42              |
| 6:g:94:ILE:HD11  | 6:g:122:LEU:HD23 | 2.01                     | 0.42              |
| 7:h:47:GLU:OE2   | 7:h:95:LEU:HD11  | 2.19                     | 0.42              |
| 8:i:16:MET:HE1   | 8:i:19:PRO:HA    | 2.01                     | 0.42              |
| 10:k:58:LEU:HD11 | 10:k:86:LEU:HD23 | 2.01                     | 0.42              |
| 30:F:29:ALA:HB3  | 30:F:30:GLU:OE1  | 2.19                     | 0.42              |
| 31:G:46:VAL:CG2  | 31:G:47:PRO:HD3  | 2.49                     | 0.42              |
| 33:I:177:MET:HE2 | 33:I:177:MET:H   | 1.84                     | 0.42              |
| 49:Y:31:ILE:O    | 49:Y:34:VAL:HG22 | 2.19                     | 0.42              |
| 50:Z:39:LYS:O    | 50:Z:40:PRO:C    | 2.62                     | 0.42              |
| 52:3:17:U:H2'    | 52:3:18:C:H6     | 1.81                     | 0.42              |
| 52:3:597:G:H2'   | 52:3:598:U:O4'   | 2.18                     | 0.42              |
| 52:3:1277:C:H2'  | 52:3:1278:G:H5'' | 2.00                     | 0.42              |
| 53:1:458:G:HO2'  | 53:1:459:U:H5    | 1.63                     | 0.42              |
| 53:1:1079:C:H2'  | 53:1:1080:A:C8   | 2.54                     | 0.42              |
| 53:1:1171:G:H2'  | 53:1:1172:C:O4'  | 2.19                     | 0.42              |
| 53:1:1437:C:H2'  | 53:1:1438:U:C6   | 2.54                     | 0.42              |
| 53:1:2819:G:H2'  | 53:1:2821:A:N7   | 2.33                     | 0.42              |
| 55:5:69:C:H2'    | 55:5:70:G:C8     | 2.54                     | 0.42              |
| 58:8:325:LYS:NZ  | 58:8:349:GLU:HA  | 2.34                     | 0.42              |
| 1:b:5:CYS:SG     | 1:b:12:ARG:NH2   | 2.92                     | 0.42              |
| 1:b:143:VAL:HG21 | 1:b:161:VAL:HG11 | 2.00                     | 0.42              |
| 1:b:216:ARG:CG   | 1:b:217:PRO:HD2  | 2.49                     | 0.42              |
| 4:e:67:THR:N     | 4:e:85:GLY:O     | 2.48                     | 0.42              |
| 8:i:102:ARG:HA   | 8:i:105:LEU:HD12 | 2.00                     | 0.42              |
| 11:l:79:LEU:HD23 | 11:l:82:LEU:HD13 | 2.01                     | 0.42              |
| 16:q:45:ALA:HB1  | 16:q:49:ARG:HH12 | 1.84                     | 0.42              |
| 20:u:80:ASP:OD2  | 20:u:95:PHE:HB3  | 2.19                     | 0.42              |
| 22:w:58:LYS:HE3  | 53:1:2366:A:H4'  | 2.01                     | 0.42              |
| 27:C:4:ILE:HG21  | 27:C:27:ARG:CZ   | 2.49                     | 0.42              |
| 30:F:11:CYS:SG   | 30:F:27:CYS:SG   | 3.17                     | 0.42              |
| 36:L:2:ARG:HB3   | 52:3:933:G:OP2   | 2.18                     | 0.42              |
| 39:O:12:ALA:HB2  | 39:O:96:VAL:HG12 | 2.01                     | 0.42              |
| 39:O:64:GLN:O    | 43:S:97:LYS:HA   | 2.19                     | 0.42              |
| 41:Q:23:LEU:O    | 41:Q:26:CYS:HB2  | 2.18                     | 0.42              |
| 42:R:6:ILE:HG13  | 42:R:7:ASN:H     | 1.83                     | 0.42              |
| 46:V:26:ARG:CZ   | 52:3:237:G:H5''  | 2.49                     | 0.42              |
| 51:a:175:ILE:HB  | 51:a:188:ASN:HB3 | 2.01                     | 0.42              |
| 52:3:41:G:H2'    | 52:3:42:G:H8     | 1.84                     | 0.42              |
| 52:3:613:C:H2'   | 52:3:614:C:C6    | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:3:911:U:H2'    | 52:3:912:C:C6     | 2.53                     | 0.42              |
| 52:3:1217:C:H2'   | 52:3:1218:C:C6    | 2.54                     | 0.42              |
| 53:1:596:U:H2'    | 53:1:597:G:C8     | 2.55                     | 0.42              |
| 53:1:633:A:H2'    | 53:1:634:C:H5'    | 2.01                     | 0.42              |
| 53:1:1709:U:O2'   | 53:1:2859:G:H1'   | 2.19                     | 0.42              |
| 53:1:2156:G:C3'   | 53:1:2157:G:H5'   | 2.49                     | 0.42              |
| 53:1:2743:U:H2'   | 53:1:2744:G:O4'   | 2.19                     | 0.42              |
| 58:8:392:VAL:C    | 58:8:393:LEU:HD22 | 2.43                     | 0.42              |
| 14:o:41:ALA:HB2   | 14:o:48:LEU:HD21  | 2.01                     | 0.42              |
| 28:D:44:VAL:HG13  | 28:D:44:VAL:O     | 2.19                     | 0.42              |
| 29:E:44:ARG:N     | 29:E:45:PRO:HD2   | 2.34                     | 0.42              |
| 30:F:15:LYS:NZ    | 53:1:2754:U:H5'   | 2.34                     | 0.42              |
| 30:F:24:ARG:NH1   | 53:1:2742:G:OP2   | 2.52                     | 0.42              |
| 32:H:110:LEU:HD22 | 32:H:203:LYS:HE3  | 2.01                     | 0.42              |
| 34:J:92:ARG:O     | 34:J:93:VAL:O     | 2.37                     | 0.42              |
| 39:O:52:LEU:HA    | 39:O:62:ARG:HG2   | 2.00                     | 0.42              |
| 40:P:85:VAL:HG22  | 40:P:92:ARG:HD2   | 2.00                     | 0.42              |
| 51:a:6:LYS:HA     | 51:a:9:ARG:HH21   | 1.84                     | 0.42              |
| 52:3:449:G:H2'    | 52:3:450:G:C8     | 2.55                     | 0.42              |
| 52:3:495:A:H4'    | 52:3:496:A:O5'    | 2.18                     | 0.42              |
| 52:3:731:G:O2'    | 52:3:732:C:H5'    | 2.20                     | 0.42              |
| 53:1:440:C:H2'    | 53:1:441:U:C6     | 2.54                     | 0.42              |
| 53:1:691:C:H2'    | 53:1:692:C:C6     | 2.54                     | 0.42              |
| 53:1:1890:A:H2'   | 53:1:1891:G:O4'   | 2.18                     | 0.42              |
| 53:1:1912:A:H62   | 53:1:1917:U:H3    | 1.67                     | 0.42              |
| 54:2:33:G:O2'     | 54:2:34:A:H5'     | 2.18                     | 0.42              |
| 57:7:76:A:O2'     | 60:7:101:PHE:C    | 2.62                     | 0.42              |
| 2:c:194:PRO:HA    | 53:1:2680:U:C5'   | 2.45                     | 0.42              |
| 3:d:150:THR:OG1   | 3:d:151:GLY:N     | 2.52                     | 0.42              |
| 8:i:89:SER:HB3    | 8:i:135:MET:HA    | 2.01                     | 0.42              |
| 17:r:51:VAL:HG23  | 17:r:52:PRO:HD2   | 2.02                     | 0.42              |
| 19:t:20:ALA:O     | 19:t:24:MET:HG2   | 2.19                     | 0.42              |
| 27:C:5:ARG:NH1    | 53:1:2285:C:OP2   | 2.51                     | 0.42              |
| 31:G:56:LEU:HD23  | 31:G:59:ILE:HD12  | 2.00                     | 0.42              |
| 52:3:1293:C:H2'   | 52:3:1294:G:C8    | 2.54                     | 0.42              |
| 52:3:1504:G:H4'   | 52:3:1505:G:O4'   | 2.19                     | 0.42              |
| 53:1:1773:A:C2'   | 53:1:1774:C:H5'   | 2.49                     | 0.42              |
| 53:1:1809:A:H2'   | 53:1:1810:A:C8    | 2.54                     | 0.42              |
| 53:1:1949:G:H2'   | 53:1:1950:G:O4'   | 2.19                     | 0.42              |
| 54:2:10:G:H2'     | 54:2:11:C:O4'     | 2.19                     | 0.42              |
| 54:2:91:C:O2'     | 54:2:92:C:H5'     | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 58:8:333:PHE:CE1  | 58:8:336:THR:HG21 | 2.55                     | 0.42              |
| 6:g:72:ILE:HD12   | 6:g:108:VAL:HG13  | 2.01                     | 0.42              |
| 8:i:15:GLY:HA2    | 8:i:50:LYS:HB3    | 2.02                     | 0.42              |
| 10:k:113:MET:SD   | 10:k:116:ILE:HD11 | 2.59                     | 0.42              |
| 11:l:2:ARG:O      | 11:l:5:THR:HG22   | 2.19                     | 0.42              |
| 33:I:131:ILE:HG12 | 52:3:620:C:C2     | 2.55                     | 0.42              |
| 37:M:94:VAL:HB    | 37:M:99:GLY:O     | 2.20                     | 0.42              |
| 40:P:58:THR:OG1   | 40:P:59:PRO:HD2   | 2.20                     | 0.42              |
| 40:P:86:LYS:HG3   | 40:P:114:PRO:HD3  | 2.02                     | 0.42              |
| 42:R:89:ARG:NH2   | 42:R:94:LEU:HD23  | 2.35                     | 0.42              |
| 52:3:314:C:H2'    | 52:3:315:A:C8     | 2.54                     | 0.42              |
| 52:3:1318:A:H2'   | 52:3:1319:A:H5'   | 2.01                     | 0.42              |
| 52:3:1347:G:O2'   | 52:3:1348:U:C5    | 2.73                     | 0.42              |
| 53:1:167:A:H2'    | 53:1:168:G:O4'    | 2.20                     | 0.42              |
| 53:1:2055:C:H2'   | 53:1:2504:U:C5'   | 2.50                     | 0.42              |
| 53:1:2087:G:H2'   | 53:1:2088:A:C8    | 2.54                     | 0.42              |
| 53:1:2098:U:H2'   | 53:1:2099:U:O4'   | 2.18                     | 0.42              |
| 53:1:2682:A:O2'   | 53:1:2683:C:H5'   | 2.20                     | 0.42              |
| 53:1:2773:C:H2'   | 53:1:2774:C:H6    | 1.85                     | 0.42              |
| 55:6:26:G:H1      | 55:6:44:A:H61     | 1.68                     | 0.42              |
| 57:7:39:U:H2'     | 57:7:40:C:C6      | 2.53                     | 0.42              |
| 58:8:215:ILE:HD12 | 58:8:228:VAL:CG2  | 2.43                     | 0.42              |
| 2:c:70:LYS:HD2    | 2:c:70:LYS:HA     | 1.83                     | 0.42              |
| 4:e:22:ASN:N      | 4:e:26:GLN:OE1    | 2.52                     | 0.42              |
| 8:i:86:LYS:HD3    | 8:i:86:LYS:HA     | 1.82                     | 0.42              |
| 12:m:42:THR:OG1   | 12:m:45:GLN:HG3   | 2.19                     | 0.42              |
| 19:t:55:VAL:HG13  | 19:t:85:VAL:HG23  | 2.02                     | 0.42              |
| 31:G:175:ALA:HB1  | 31:G:180:ILE:HB   | 2.02                     | 0.42              |
| 32:H:188:ALA:HB3  | 32:H:195:ILE:HB   | 2.01                     | 0.42              |
| 34:J:24:VAL:HG12  | 34:J:25:LYS:N     | 2.34                     | 0.42              |
| 52:3:823:C:H2'    | 52:3:824:G:C8     | 2.54                     | 0.42              |
| 52:3:1494:G:O2'   | 52:3:1495:U:H5'   | 2.20                     | 0.42              |
| 52:3:1497:G:H2'   | 52:3:1498:U:H5'   | 2.02                     | 0.42              |
| 53:1:708:G:O2'    | 53:1:709:U:H5'    | 2.19                     | 0.42              |
| 53:1:1140:C:C2'   | 53:1:1141:U:H5'   | 2.50                     | 0.42              |
| 53:1:1324:G:H4'   | 53:1:1616:A:N7    | 2.35                     | 0.42              |
| 53:1:1991:U:H2'   | 53:1:1992:G:C5'   | 2.48                     | 0.42              |
| 53:1:2162:G:H2'   | 53:1:2163:A:H8    | 1.83                     | 0.42              |
| 55:6:37:A:H2'     | 55:6:38:A:O4'     | 2.20                     | 0.42              |
| 1:b:216:ARG:HG3   | 1:b:217:PRO:HD2   | 2.02                     | 0.42              |
| 6:g:47:PHE:HA     | 6:g:51:ARG:HB2    | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:i:7:TYR:HA     | 8:i:58:ILE:O     | 2.20                     | 0.42              |
| 12:m:75:GLU:CD   | 53:1:957:C:H5'   | 2.44                     | 0.42              |
| 14:o:11:ALA:HB2  | 14:o:96:GLY:N    | 2.35                     | 0.42              |
| 22:w:67:VAL:HG22 | 22:w:67:VAL:O    | 2.19                     | 0.42              |
| 34:J:158:LYS:HD3 | 34:J:158:LYS:N   | 2.34                     | 0.42              |
| 35:K:17:GLN:O    | 35:K:17:GLN:HG2  | 2.20                     | 0.42              |
| 36:L:115:MET:HA  | 36:L:118:ARG:HE  | 1.84                     | 0.42              |
| 40:P:52:ARG:NH1  | 52:3:689:C:OP2   | 2.53                     | 0.42              |
| 50:Z:36:PHE:C    | 50:Z:38:GLU:H    | 2.28                     | 0.42              |
| 52:3:1130:A:H61  | 52:3:1144:G:H1'  | 1.83                     | 0.42              |
| 52:3:1340:A:H2'  | 52:3:1341:U:O4'  | 2.20                     | 0.42              |
| 53:1:217:A:H2'   | 53:1:218:A:O4'   | 2.19                     | 0.42              |
| 53:1:722:A:H2'   | 53:1:723:C:C6    | 2.55                     | 0.42              |
| 53:1:728:G:H3'   | 53:1:729:G:H5'   | 2.01                     | 0.42              |
| 53:1:1434:A:H2'  | 53:1:1435:G:H8   | 1.83                     | 0.42              |
| 53:1:1564:C:H2'  | 53:1:1565:C:O4'  | 2.19                     | 0.42              |
| 53:1:1721:G:H1'  | 53:1:1739:A:H61  | 1.84                     | 0.42              |
| 53:1:2512:C:H2'  | 53:1:2513:A:C4'  | 2.49                     | 0.42              |
| 54:2:60:C:H2'    | 54:2:61:G:C8     | 2.55                     | 0.42              |
| 57:7:68:C:H2'    | 57:7:69:G:H8     | 1.85                     | 0.42              |
| 1:b:269:ARG:HA   | 1:b:269:ARG:HD2  | 1.69                     | 0.42              |
| 3:d:170:ARG:NH2  | 3:d:176:ASP:OD1  | 2.53                     | 0.42              |
| 4:e:23:SER:OG    | 4:e:26:GLN:HB2   | 2.20                     | 0.42              |
| 7:h:117:LEU:CD2  | 7:h:120:ALA:HA   | 2.50                     | 0.42              |
| 8:i:30:GLN:HG2   | 8:i:60:VAL:HG21  | 2.01                     | 0.42              |
| 15:p:1:SER:OG    | 15:p:2:ASN:N     | 2.51                     | 0.42              |
| 20:u:3:LYS:HB3   | 20:u:4:ILE:HD12  | 2.02                     | 0.42              |
| 21:v:42:LEU:HD13 | 21:v:47:VAL:HG21 | 2.02                     | 0.42              |
| 27:C:41:VAL:HG23 | 27:C:42:VAL:HG23 | 2.01                     | 0.42              |
| 27:C:46:VAL:HG12 | 27:C:47:ILE:N    | 2.34                     | 0.42              |
| 28:D:16:HIS:ND1  | 53:1:465:G:H4'   | 2.35                     | 0.42              |
| 30:F:12:ARG:HH22 | 53:1:1102:C:C1'  | 2.33                     | 0.42              |
| 31:G:46:VAL:O    | 31:G:50:ASN:ND2  | 2.51                     | 0.42              |
| 31:G:94:ARG:NH1  | 52:3:1101:A:OP2  | 2.53                     | 0.42              |
| 35:K:2:ARG:HD3   | 35:K:91:ARG:HH22 | 1.84                     | 0.42              |
| 38:N:4:GLN:HA    | 38:N:21:LYS:HG2  | 2.02                     | 0.42              |
| 38:N:29:ILE:HA   | 38:N:64:ILE:O    | 2.20                     | 0.42              |
| 39:O:10:LEU:HD23 | 39:O:10:LEU:N    | 2.34                     | 0.42              |
| 40:P:25:SER:O    | 40:P:89:GLY:HA2  | 2.20                     | 0.42              |
| 43:S:76:PHE:CD2  | 43:S:83:VAL:HG21 | 2.55                     | 0.42              |
| 51:a:219:GLY:O   | 53:1:2176:A:H5'  | 2.20                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 52:3:663:A:H5'    | 52:3:836:G:OP1   | 2.19                     | 0.42              |
| 52:3:917:G:H2'    | 52:3:918:A:C8    | 2.54                     | 0.42              |
| 52:3:1005:A:H2'   | 52:3:1006:G:O4'  | 2.20                     | 0.42              |
| 52:3:1162:C:H2'   | 52:3:1163:A:C8   | 2.55                     | 0.42              |
| 53:1:1106:G:H2'   | 53:1:1107:G:O4'  | 2.20                     | 0.42              |
| 53:1:1388:G:H2'   | 53:1:1389:G:H8   | 1.84                     | 0.42              |
| 53:1:1388:G:H2'   | 53:1:1389:G:C8   | 2.55                     | 0.42              |
| 53:1:2282:G:H4'   | 53:1:2389:G:O2'  | 2.20                     | 0.42              |
| 53:1:2777:G:H1'   | 53:1:2779:U:H5   | 1.85                     | 0.42              |
| 5:f:97:VAL:HG23   | 5:f:124:CYS:SG   | 2.60                     | 0.42              |
| 23:x:71:ARG:NH1   | 23:x:77:TYR:OH   | 2.53                     | 0.42              |
| 24:y:32:ALA:HB2   | 24:y:37:LEU:HD23 | 2.01                     | 0.42              |
| 31:G:116:LEU:HD12 | 31:G:116:LEU:HA  | 1.90                     | 0.42              |
| 31:G:205:ALA:HB3  | 31:G:208:ALA:HB2 | 2.02                     | 0.42              |
| 35:K:13:ASP:OD1   | 35:K:13:ASP:N    | 2.51                     | 0.42              |
| 37:M:31:LEU:HD13  | 52:3:643:C:H5'   | 2.02                     | 0.42              |
| 53:1:11:C:H3'     | 53:1:12:U:H5''   | 2.01                     | 0.42              |
| 53:1:438:G:H2'    | 53:1:439:A:C8    | 2.55                     | 0.42              |
| 53:1:819:A:H2'    | 53:1:820:A:O4'   | 2.20                     | 0.42              |
| 53:1:1170:C:H2'   | 53:1:1171:G:C8   | 2.55                     | 0.42              |
| 53:1:2707:U:H2'   | 53:1:2708:G:H8   | 1.84                     | 0.42              |
| 53:1:2875:C:H2'   | 53:1:2876:G:C8   | 2.55                     | 0.42              |
| 6:g:29:PHE:HB2    | 53:1:2198:A:C2   | 2.55                     | 0.42              |
| 7:h:67:THR:N      | 7:h:68:PRO:CD    | 2.83                     | 0.42              |
| 21:v:80:HIS:CE1   | 21:v:81:PRO:HD2  | 2.55                     | 0.42              |
| 31:G:114:LYS:HA   | 31:G:117:GLU:CD  | 2.45                     | 0.42              |
| 38:N:33:SER:H     | 38:N:36:GLN:CD   | 2.27                     | 0.42              |
| 43:S:45:LEU:HG    | 48:X:12:LEU:HD11 | 2.02                     | 0.42              |
| 48:X:40:PHE:HA    | 48:X:41:PRO:HD3  | 1.92                     | 0.42              |
| 52:3:458:U:H2'    | 52:3:459:A:H8    | 1.85                     | 0.42              |
| 52:3:1245:C:H2'   | 52:3:1246:A:H8   | 1.84                     | 0.42              |
| 52:3:1514:G:O2'   | 52:3:1515:G:H5'  | 2.20                     | 0.42              |
| 53:1:481:G:H1'    | 53:1:506:G:N2    | 2.35                     | 0.42              |
| 53:1:828:U:H2'    | 53:1:829:A:C8    | 2.55                     | 0.42              |
| 53:1:1086:A:H3'   | 53:1:1086:A:N3   | 2.35                     | 0.42              |
| 53:1:1179:G:N7    | 53:1:1180:U:H1'  | 2.34                     | 0.42              |
| 53:1:1219:U:H2'   | 53:1:1220:G:C8   | 2.55                     | 0.42              |
| 53:1:1463:C:H2'   | 53:1:1464:G:C8   | 2.55                     | 0.42              |
| 53:1:1779:U:H5    | 53:1:1784:A:N7   | 2.17                     | 0.42              |
| 53:1:2030:A:H4'   | 53:1:2031:A:C8   | 2.55                     | 0.42              |
| 53:1:2294:G:H2'   | 53:1:2295:C:C6   | 2.55                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 54:2:3:C:C3'     | 54:2:4:C:C5'      | 2.97                     | 0.42              |
| 55:6:22:G:O2'    | 55:6:23:C:H5'     | 2.19                     | 0.42              |
| 57:7:26:A:H61    | 57:7:45:U:H3      | 1.68                     | 0.42              |
| 2:c:5:VAL:H      | 2:c:32:ASN:ND2    | 1.95                     | 0.41              |
| 5:f:155:PRO:HG3  | 53:1:2530:A:N6    | 2.35                     | 0.41              |
| 8:i:89:SER:HB2   | 8:i:92:PRO:HG3    | 2.02                     | 0.41              |
| 15:p:95:LYS:HB3  | 15:p:97:TYR:CD2   | 2.55                     | 0.41              |
| 20:u:93:ARG:HB2  | 20:u:102:ILE:HD12 | 2.02                     | 0.41              |
| 33:I:70:GLN:HG3  | 52:3:402:G:OP1    | 2.20                     | 0.41              |
| 41:Q:66:ILE:HG21 | 41:Q:71:HIS:CD2   | 2.55                     | 0.41              |
| 51:a:53:ARG:O    | 55:6:62:C:H4'     | 2.18                     | 0.41              |
| 52:3:593:U:H2'   | 52:3:594:U:C6     | 2.55                     | 0.41              |
| 52:3:1084:G:H5'  | 52:3:1102:A:OP2   | 2.20                     | 0.41              |
| 52:3:1427:C:H2'  | 52:3:1428:A:H8    | 1.85                     | 0.41              |
| 53:1:274:C:H2'   | 53:1:275:C:O4'    | 2.20                     | 0.41              |
| 53:1:552:U:H2'   | 53:1:553:G:C8     | 2.55                     | 0.41              |
| 53:1:744:U:H5''  | 53:1:1658:C:H5''  | 2.02                     | 0.41              |
| 53:1:825:A:H2'   | 53:1:826:U:C6     | 2.55                     | 0.41              |
| 53:1:1280:G:O2'  | 53:1:1281:G:H5'   | 2.20                     | 0.41              |
| 53:1:1636:U:H2'  | 53:1:1637:A:C8    | 2.55                     | 0.41              |
| 53:1:1833:C:O2'  | 53:1:1834:U:H5'   | 2.19                     | 0.41              |
| 53:1:2343:U:H2'  | 53:1:2344:U:C6    | 2.55                     | 0.41              |
| 53:1:2514:U:O2'  | 53:1:2515:C:H5'   | 2.20                     | 0.41              |
| 53:1:2553:G:H1'  | 53:1:2582:G:H21   | 1.85                     | 0.41              |
| 53:1:2724:U:H2'  | 53:1:2725:A:C8    | 2.55                     | 0.41              |
| 55:6:59:A:C2'    | 55:6:60:U:H5'     | 2.49                     | 0.41              |
| 3:d:76:PRO:HA    | 3:d:82:GLY:HA2    | 2.01                     | 0.41              |
| 4:e:32:LYS:HG2   | 4:e:156:THR:CG2   | 2.50                     | 0.41              |
| 5:f:174:LYS:HD3  | 53:1:2531:A:P     | 2.60                     | 0.41              |
| 8:i:11:GLN:OE1   | 8:i:56:VAL:HG13   | 2.20                     | 0.41              |
| 9:j:120:ARG:NE   | 53:1:2780:G:OP2   | 2.52                     | 0.41              |
| 14:o:30:ARG:NH1  | 54:2:49:C:OP2     | 2.51                     | 0.41              |
| 20:u:14:THR:OG1  | 20:u:68:ASN:ND2   | 2.53                     | 0.41              |
| 24:y:2:LYS:HG3   | 24:y:3:ALA:N      | 2.35                     | 0.41              |
| 24:y:23:ARG:HB3  | 24:y:24:GLU:H     | 1.64                     | 0.41              |
| 32:H:54:ILE:HD12 | 32:H:67:ILE:HG13  | 2.02                     | 0.41              |
| 33:I:7:LYS:HG2   | 52:3:430:A:OP2    | 2.20                     | 0.41              |
| 33:I:84:ASN:CG   | 33:I:87:GLU:HG2   | 2.45                     | 0.41              |
| 37:M:17:GLN:HG3  | 37:M:71:VAL:HB    | 2.01                     | 0.41              |
| 44:T:23:SER:OG   | 44:T:26:VAL:HG23  | 2.20                     | 0.41              |
| 52:3:323:U:H2'   | 52:3:324:G:O4'    | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 52:3:735:C:H2'   | 52:3:736:C:C6     | 2.55                     | 0.41              |
| 52:3:817:C:H4'   | 52:3:818:G:H5''   | 2.01                     | 0.41              |
| 52:3:1038:C:H2'  | 52:3:1039:G:H8    | 1.85                     | 0.41              |
| 53:1:171:U:H2'   | 53:1:172:A:C8     | 2.54                     | 0.41              |
| 53:1:371:A:H61   | 53:1:401:A:H3'    | 1.85                     | 0.41              |
| 53:1:634:C:H2'   | 53:1:635:C:C6     | 2.54                     | 0.41              |
| 53:1:680:C:H2'   | 53:1:681:G:C8     | 2.55                     | 0.41              |
| 53:1:942:G:H2'   | 53:1:943:A:O4'    | 2.20                     | 0.41              |
| 53:1:1098:A:H2'  | 53:1:1099:G:O4'   | 2.20                     | 0.41              |
| 53:1:1635:A:H2'  | 53:1:1636:U:O4'   | 2.19                     | 0.41              |
| 53:1:2026:U:H2'  | 53:1:2027:G:C8    | 2.55                     | 0.41              |
| 53:1:2297:A:N1   | 53:1:2321:U:H5    | 2.18                     | 0.41              |
| 53:1:2591:C:H2'  | 53:1:2592:G:H8    | 1.85                     | 0.41              |
| 53:1:2709:G:H2'  | 53:1:2710:C:C6    | 2.55                     | 0.41              |
| 58:8:18:ILE:HG13 | 58:8:104:LEU:HD23 | 2.02                     | 0.41              |
| 3:d:144:GLU:HG2  | 3:d:145:ASP:H     | 1.85                     | 0.41              |
| 4:e:88:VAL:HA    | 54:2:42:C:O2      | 2.20                     | 0.41              |
| 15:p:96:LEU:HD22 | 15:p:96:LEU:N     | 2.34                     | 0.41              |
| 31:G:5:MET:SD    | 31:G:46:VAL:HG11  | 2.60                     | 0.41              |
| 35:K:3:HIS:O     | 35:K:92:THR:HG22  | 2.20                     | 0.41              |
| 36:L:136:LYS:HA  | 36:L:139:ASP:OD2  | 2.20                     | 0.41              |
| 37:M:17:GLN:HE21 | 37:M:71:VAL:H     | 1.69                     | 0.41              |
| 42:R:100:ARG:NH1 | 52:3:950:U:C6     | 2.88                     | 0.41              |
| 44:T:88:ARG:HD3  | 44:T:88:ARG:N     | 2.36                     | 0.41              |
| 46:V:69:THR:OG1  | 46:V:70:LYS:N     | 2.52                     | 0.41              |
| 50:Z:3:ILE:HG22  | 50:Z:3:ILE:O      | 2.21                     | 0.41              |
| 52:3:7:A:H5'     | 52:3:298:A:H5'    | 2.03                     | 0.41              |
| 52:3:40:C:O2'    | 52:3:41:G:H5'     | 2.20                     | 0.41              |
| 52:3:923:A:H61   | 52:3:1393:U:H3    | 1.67                     | 0.41              |
| 52:3:955:U:H3    | 52:3:1225:A:N6    | 2.07                     | 0.41              |
| 52:3:1033:G:C2'  | 52:3:1034:G:H5''  | 2.48                     | 0.41              |
| 52:3:1401:G:H2'  | 52:3:1402:C:O4'   | 2.19                     | 0.41              |
| 53:1:56:A:H2'    | 53:1:57:C:O4'     | 2.20                     | 0.41              |
| 53:1:214:G:O2'   | 53:1:215:G:H5'    | 2.21                     | 0.41              |
| 53:1:1760:C:H2'  | 53:1:1761:C:H5'   | 2.01                     | 0.41              |
| 53:1:2391:G:H4'  | 53:1:2392:A:OP1   | 2.20                     | 0.41              |
| 53:1:2678:C:H2'  | 53:1:2679:A:O4'   | 2.20                     | 0.41              |
| 53:1:2713:U:H3'  | 53:1:2714:G:H5''  | 2.01                     | 0.41              |
| 54:2:88:C:H5''   | 54:2:89:U:OP1     | 2.20                     | 0.41              |
| 58:8:10:LYS:HB2  | 58:8:76:HIS:HB2   | 2.03                     | 0.41              |
| 1:b:96:LYS:HD2   | 1:b:96:LYS:HA     | 1.81                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:d:152:GLU:OE2   | 3:d:154:ASP:HB3  | 2.21                     | 0.41              |
| 4:e:132:ARG:HG2   | 4:e:133:GLU:OE2  | 2.21                     | 0.41              |
| 5:f:82:PHE:CE2    | 5:f:137:LYS:HB2  | 2.54                     | 0.41              |
| 7:h:31:ARG:HH21   | 53:1:1054:A:H4'  | 1.86                     | 0.41              |
| 7:h:108:VAL:HG13  | 7:h:109:LYS:N    | 2.35                     | 0.41              |
| 8:i:73:PRO:HA     | 8:i:74:PRO:HD3   | 1.94                     | 0.41              |
| 10:k:40:LYS:NZ    | 10:k:89:ASN:OD1  | 2.42                     | 0.41              |
| 11:l:64:PHE:N     | 11:l:64:PHE:CD1  | 2.88                     | 0.41              |
| 18:s:25:ARG:NH2   | 18:s:74:ILE:O    | 2.53                     | 0.41              |
| 24:y:41:HIS:CG    | 53:1:96:C:H4'    | 2.55                     | 0.41              |
| 24:y:42:LEU:O     | 24:y:46:VAL:HG23 | 2.20                     | 0.41              |
| 36:L:63:VAL:HA    | 36:L:66:GLU:HG2  | 2.02                     | 0.41              |
| 40:P:107:THR:HG23 | 40:P:108:ASN:OD1 | 2.21                     | 0.41              |
| 44:T:50:HIS:ND1   | 52:3:667:G:H4'   | 2.35                     | 0.41              |
| 44:T:76:ARG:HA    | 44:T:79:GLN:HB2  | 2.01                     | 0.41              |
| 50:Z:67:THR:C     | 52:3:1167:A:C8   | 2.98                     | 0.41              |
| 52:3:212:G:O2'    | 52:3:213:G:H5'   | 2.20                     | 0.41              |
| 52:3:291:U:O2'    | 52:3:292:G:H5'   | 2.21                     | 0.41              |
| 52:3:570:G:O2'    | 52:3:819:A:H2'   | 2.19                     | 0.41              |
| 52:3:1014:A:C2    | 52:3:1219:A:H1'  | 2.54                     | 0.41              |
| 53:1:67:U:H2'     | 53:1:68:G:H8     | 1.84                     | 0.41              |
| 53:1:635:C:H2'    | 53:1:636:G:H8    | 1.82                     | 0.41              |
| 53:1:765:C:H2'    | 53:1:766:U:C6    | 2.55                     | 0.41              |
| 53:1:1086:A:H4'   | 53:1:1103:A:N1   | 2.35                     | 0.41              |
| 53:1:1911:U:H2'   | 53:1:1918:A:N1   | 2.35                     | 0.41              |
| 58:8:158:LEU:HD22 | 58:8:165:GLY:HA2 | 2.02                     | 0.41              |
| 58:8:322:PRO:HG2  | 58:8:350:MET:HE2 | 2.02                     | 0.41              |
| 3:d:52:VAL:HG13   | 53:1:452:G:OP1   | 2.20                     | 0.41              |
| 3:d:148:ILE:HD13  | 3:d:187:VAL:CG2  | 2.50                     | 0.41              |
| 3:d:154:ASP:OD1   | 3:d:154:ASP:N    | 2.52                     | 0.41              |
| 6:g:15:LEU:HD21   | 6:g:56:ALA:HB1   | 2.01                     | 0.41              |
| 10:k:59:LYS:HG3   | 10:k:89:ASN:HA   | 2.02                     | 0.41              |
| 32:H:137:VAL:HG12 | 32:H:169:GLU:OE2 | 2.20                     | 0.41              |
| 36:L:105:GLU:HA   | 36:L:108:ARG:HG2 | 2.01                     | 0.41              |
| 38:N:6:TYR:OH     | 38:N:8:THR:HG22  | 2.21                     | 0.41              |
| 38:N:58:GLU:H     | 38:N:59:LYS:HD2  | 1.85                     | 0.41              |
| 43:S:53:ASP:HB3   | 43:S:54:SER:H    | 1.73                     | 0.41              |
| 45:U:50:THR:HG23  | 45:U:52:LEU:HD23 | 2.03                     | 0.41              |
| 45:U:63:GLN:HE21  | 52:3:228:A:H5'   | 1.85                     | 0.41              |
| 51:a:190:GLU:O    | 51:a:193:LEU:HG  | 2.19                     | 0.41              |
| 52:3:355:C:H2'    | 52:3:356:A:O4'   | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:3:601:G:H2'    | 52:3:602:A:C8     | 2.55                     | 0.41              |
| 52:3:893:C:H2'    | 52:3:894:G:H8     | 1.85                     | 0.41              |
| 52:3:1010:U:H2'   | 52:3:1011:C:C6    | 2.55                     | 0.41              |
| 52:3:1225:A:H2'   | 52:3:1225:A:N3    | 2.36                     | 0.41              |
| 53:1:20:C:H2'     | 53:1:21:A:H8      | 1.85                     | 0.41              |
| 53:1:39:G:H2'     | 53:1:40:U:C6      | 2.55                     | 0.41              |
| 53:1:547:A:H3'    | 53:1:547:A:N3     | 2.35                     | 0.41              |
| 53:1:925:A:H2'    | 53:1:926:G:C8     | 2.56                     | 0.41              |
| 53:1:1071:G:O2'   | 53:1:1089:A:H2'   | 2.21                     | 0.41              |
| 53:1:2008:C:H2'   | 53:1:2009:A:H8    | 1.85                     | 0.41              |
| 53:1:2069:G:O2'   | 53:1:2070:A:H5'   | 2.20                     | 0.41              |
| 53:1:2588:G:C2'   | 53:1:2589:A:H5'   | 2.50                     | 0.41              |
| 53:1:2741:A:H2'   | 53:1:2742:G:H5'   | 2.01                     | 0.41              |
| 58:8:117:ARG:HH22 | 58:8:160:GLN:NE2  | 2.18                     | 0.41              |
| 58:8:118:GLU:OE2  | 58:8:122:LEU:HD11 | 2.21                     | 0.41              |
| 3:d:149:ILE:HG21  | 3:d:188:MET:HG2   | 2.02                     | 0.41              |
| 4:e:114:ARG:HG3   | 4:e:177:ARG:HD3   | 2.02                     | 0.41              |
| 5:f:159:LYS:HE2   | 53:1:2658:C:H5'   | 2.03                     | 0.41              |
| 7:h:28:ALA:CB     | 7:h:109:LYS:HE3   | 2.51                     | 0.41              |
| 10:k:71:ARG:NH1   | 10:k:106:GLU:OE2  | 2.54                     | 0.41              |
| 25:z:20:LYS:HE2   | 25:z:20:LYS:HB3   | 1.84                     | 0.41              |
| 32:H:111:ASP:OD2  | 32:H:114:LEU:HD23 | 2.21                     | 0.41              |
| 40:P:67:GLU:O     | 40:P:70:ALA:HB3   | 2.20                     | 0.41              |
| 41:Q:53:ARG:HA    | 41:Q:63:THR:HA    | 2.01                     | 0.41              |
| 43:S:4:SER:CB     | 52:3:1216:A:H5''  | 2.50                     | 0.41              |
| 46:V:48:GLU:HB3   | 46:V:51:GLU:CD    | 2.46                     | 0.41              |
| 52:3:352:C:H4'    | 52:3:354:G:OP1    | 2.21                     | 0.41              |
| 52:3:1070:U:O2'   | 52:3:1071:C:H5'   | 2.21                     | 0.41              |
| 52:3:1409:C:H2'   | 52:3:1410:A:C8    | 2.56                     | 0.41              |
| 52:3:1436:U:H2'   | 52:3:1437:A:C8    | 2.55                     | 0.41              |
| 53:1:594:U:H2'    | 53:1:595:C:C6     | 2.54                     | 0.41              |
| 53:1:610:C:H2'    | 53:1:611:C:C6     | 2.55                     | 0.41              |
| 53:1:873:C:H2'    | 53:1:874:G:H8     | 1.86                     | 0.41              |
| 53:1:906:U:H2'    | 53:1:907:G:C5'    | 2.37                     | 0.41              |
| 53:1:948:C:H2'    | 53:1:949:G:H8     | 1.85                     | 0.41              |
| 53:1:953:G:O2'    | 53:1:954:G:H5'    | 2.21                     | 0.41              |
| 53:1:1086:A:H1'   | 53:1:1103:A:H61   | 1.85                     | 0.41              |
| 53:1:1354:A:H2'   | 53:1:1355:G:O4'   | 2.20                     | 0.41              |
| 53:1:1494:A:H2'   | 53:1:1495:A:H8    | 1.85                     | 0.41              |
| 53:1:1598:A:N3    | 53:1:1598:A:H2'   | 2.36                     | 0.41              |
| 53:1:1680:U:C2'   | 53:1:1681:G:H5'   | 2.50                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:1:2128:G:H2'  | 53:1:2129:C:O4'   | 2.20                     | 0.41              |
| 53:1:2144:G:H1'  | 53:1:2147:A:H61   | 1.85                     | 0.41              |
| 53:1:2526:G:H2'  | 53:1:2527:C:C6    | 2.55                     | 0.41              |
| 53:1:2586:U:O2'  | 53:1:2587:A:H5'   | 2.20                     | 0.41              |
| 58:8:5:LYS:HD3   | 58:8:265:LEU:CB   | 2.45                     | 0.41              |
| 58:8:305:PHE:HA  | 58:8:393:LEU:HD23 | 2.02                     | 0.41              |
| 3:d:176:ASP:OD1  | 3:d:179:SER:OG    | 2.35                     | 0.41              |
| 5:f:44:HIS:CG    | 5:f:45:ALA:H      | 2.38                     | 0.41              |
| 9:j:69:ARG:HA    | 9:j:89:PHE:HD2    | 1.85                     | 0.41              |
| 13:n:90:ARG:NH2  | 53:1:2880:C:O2'   | 2.45                     | 0.41              |
| 14:o:34:HIS:CE1  | 14:o:54:VAL:HA    | 2.56                     | 0.41              |
| 24:y:51:ALA:HA   | 53:1:72:U:O4'     | 2.20                     | 0.41              |
| 33:I:96:ARG:O    | 33:I:100:VAL:HG23 | 2.21                     | 0.41              |
| 36:L:63:VAL:O    | 36:L:67:ASN:ND2   | 2.54                     | 0.41              |
| 38:N:23:GLY:HA3  | 38:N:61:ASP:OD2   | 2.20                     | 0.41              |
| 42:R:102:LYS:HG3 | 52:3:1226:C:C4    | 2.55                     | 0.41              |
| 50:Z:67:THR:OXT  | 52:3:1167:A:C8    | 2.73                     | 0.41              |
| 52:3:434:U:H2'   | 52:3:435:A:H8     | 1.86                     | 0.41              |
| 52:3:458:U:H2'   | 52:3:459:A:C8     | 2.56                     | 0.41              |
| 52:3:893:C:H2'   | 52:3:894:G:C8     | 2.56                     | 0.41              |
| 52:3:1301:U:O2   | 52:3:1301:U:H2'   | 2.21                     | 0.41              |
| 53:1:6:A:H2'     | 53:1:7:G:C8       | 2.56                     | 0.41              |
| 53:1:57:C:H2'    | 53:1:58:G:O4'     | 2.20                     | 0.41              |
| 53:1:75:G:H22    | 53:1:111:A:H2     | 1.67                     | 0.41              |
| 53:1:1125:G:C6   | 53:1:1126:A:N6    | 2.89                     | 0.41              |
| 53:1:1433:A:H2'  | 53:1:1434:A:C8    | 2.56                     | 0.41              |
| 53:1:1629:U:H2'  | 53:1:1630:A:C8    | 2.56                     | 0.41              |
| 53:1:2559:C:O2'  | 53:1:2560:A:H5'   | 2.20                     | 0.41              |
| 53:1:2652:C:H2'  | 53:1:2653:U:O4'   | 2.20                     | 0.41              |
| 53:1:2801:G:H2'  | 53:1:2802:G:H8    | 1.82                     | 0.41              |
| 1:b:50:THR:HG21  | 53:1:1814:G:H4'   | 2.03                     | 0.41              |
| 1:b:66:PHE:O     | 1:b:68:ARG:HG2    | 2.21                     | 0.41              |
| 1:b:257:ARG:HD3  | 53:1:1799:G:OP1   | 2.20                     | 0.41              |
| 4:e:162:ASP:OD1  | 4:e:162:ASP:N     | 2.54                     | 0.41              |
| 8:i:48:ILE:HG12  | 8:i:49:GLU:H      | 1.86                     | 0.41              |
| 8:i:126:ARG:HA   | 8:i:129:GLU:HG3   | 2.03                     | 0.41              |
| 9:j:56:VAL:HB    | 9:j:124:VAL:HG12  | 2.01                     | 0.41              |
| 19:t:59:ASN:O    | 19:t:84:TYR:N     | 2.53                     | 0.41              |
| 25:z:51:SER:HA   | 25:z:54:VAL:HG22  | 2.03                     | 0.41              |
| 28:D:18:PHE:HB2  | 28:D:43:THR:HG21  | 2.02                     | 0.41              |
| 28:D:26:ASN:HB3  | 53:1:682:G:H5'    | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:H:86:LEU:O     | 32:H:90:VAL:HG22  | 2.21                     | 0.41              |
| 32:H:155:ARG:HG3  | 32:H:192:TYR:O    | 2.21                     | 0.41              |
| 32:H:187:GLU:OE1  | 32:H:187:GLU:N    | 2.54                     | 0.41              |
| 33:I:146:GLU:HA   | 33:I:149:LYS:HE2  | 2.03                     | 0.41              |
| 36:L:41:ILE:HD13  | 36:L:115:MET:HB3  | 2.03                     | 0.41              |
| 36:L:128:GLU:HG2  | 36:L:130:LYS:HG2  | 2.02                     | 0.41              |
| 39:O:71:LEU:N     | 39:O:71:LEU:HD12  | 2.36                     | 0.41              |
| 52:3:225:C:H3'    | 52:3:226:G:H5''   | 2.00                     | 0.41              |
| 52:3:424:G:H2'    | 52:3:425:G:H8     | 1.85                     | 0.41              |
| 52:3:783:C:H2'    | 52:3:784:A:H8     | 1.85                     | 0.41              |
| 52:3:1367:C:H2'   | 52:3:1368:A:C8    | 2.56                     | 0.41              |
| 53:1:568:U:H2'    | 53:1:570:G:OP2    | 2.19                     | 0.41              |
| 53:1:779:U:H2'    | 53:1:780:G:O4'    | 2.20                     | 0.41              |
| 53:1:1188:U:O2'   | 53:1:1189:A:H5'   | 2.21                     | 0.41              |
| 53:1:2480:C:H2'   | 53:1:2481:G:O4'   | 2.21                     | 0.41              |
| 53:1:2514:U:H2'   | 53:1:2515:C:H6    | 1.84                     | 0.41              |
| 54:2:55:U:O2'     | 54:2:56:G:H5'     | 2.21                     | 0.41              |
| 55:6:9:G:H1'      | 55:6:45:G:H2'     | 2.02                     | 0.41              |
| 58:8:185:TRP:O    | 58:8:188:LYS:HB2  | 2.20                     | 0.41              |
| 3:d:50:ALA:HB2    | 53:1:801:G:C8     | 2.55                     | 0.41              |
| 6:g:83:LYS:HD3    | 6:g:84:ALA:N      | 2.36                     | 0.41              |
| 7:h:118:ILE:HD13  | 7:h:118:ILE:HA    | 1.89                     | 0.41              |
| 13:n:56:LYS:NZ    | 13:n:87:PHE:O     | 2.53                     | 0.41              |
| 14:o:80:GLU:OE2   | 14:o:81:ARG:NE    | 2.49                     | 0.41              |
| 14:o:115:LEU:HD12 | 14:o:115:LEU:HA   | 1.95                     | 0.41              |
| 15:p:77:SER:OG    | 15:p:79:VAL:HG12  | 2.21                     | 0.41              |
| 17:r:6:GLN:OE1    | 17:r:11:GLN:NE2   | 2.54                     | 0.41              |
| 19:t:5:GLU:O      | 19:t:9:LYS:HD3    | 2.20                     | 0.41              |
| 20:u:40:LEU:HD22  | 20:u:59:GLU:HG3   | 2.03                     | 0.41              |
| 21:v:75:GLN:N     | 21:v:90:ASP:O     | 2.48                     | 0.41              |
| 24:y:9:LYS:NZ     | 24:y:11:VAL:HB    | 2.33                     | 0.41              |
| 24:y:24:GLU:O     | 24:y:25:GLN:C     | 2.63                     | 0.41              |
| 25:z:8:GLN:NE2    | 25:z:23:LEU:HD13  | 2.36                     | 0.41              |
| 27:C:4:ILE:HD13   | 27:C:27:ARG:NH2   | 2.36                     | 0.41              |
| 31:G:4:SER:OG     | 31:G:5:MET:N      | 2.54                     | 0.41              |
| 32:H:123:LEU:O    | 32:H:123:LEU:HD23 | 2.20                     | 0.41              |
| 33:I:36:ALA:HA    | 33:I:41:GLY:HA3   | 2.02                     | 0.41              |
| 35:K:10:VAL:HG12  | 35:K:58:HIS:HB3   | 2.03                     | 0.41              |
| 35:K:18:VAL:HG23  | 35:K:19:PRO:HD3   | 2.03                     | 0.41              |
| 35:K:67:PRO:HG2   | 35:K:70:VAL:HG12  | 2.03                     | 0.41              |
| 37:M:7:ALA:O      | 37:M:10:LEU:HG    | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:M:14:ARG:HD2   | 52:3:875:U:O2'    | 2.21                     | 0.41              |
| 38:N:6:TYR:O      | 38:N:85:ALA:HA    | 2.21                     | 0.41              |
| 38:N:11:ARG:HA    | 38:N:105:ARG:NH1  | 2.35                     | 0.41              |
| 38:N:17:ARG:NH1   | 52:3:1129:C:H4'   | 2.34                     | 0.41              |
| 38:N:119:LYS:HD2  | 52:3:1350:A:OP2   | 2.20                     | 0.41              |
| 40:P:115:ILE:HD11 | 50:Z:27:VAL:HG22  | 2.03                     | 0.41              |
| 45:U:56:ARG:HD2   | 45:U:56:ARG:HA    | 1.91                     | 0.41              |
| 46:V:48:GLU:O     | 46:V:49:ASN:C     | 2.64                     | 0.41              |
| 49:Y:17:ARG:HH11  | 49:Y:17:ARG:HG3   | 1.86                     | 0.41              |
| 52:3:50:A:H4'     | 52:3:51:A:H5'     | 2.03                     | 0.41              |
| 52:3:766:A:H62    | 52:3:813:U:H3     | 1.68                     | 0.41              |
| 53:1:210:C:H2'    | 53:1:211:C:C6     | 2.55                     | 0.41              |
| 53:1:511:U:C2'    | 53:1:512:G:H5'    | 2.51                     | 0.41              |
| 53:1:1326:U:H2'   | 53:1:1327:A:H8    | 1.86                     | 0.41              |
| 53:1:1461:C:H2'   | 53:1:1462:C:C6    | 2.56                     | 0.41              |
| 53:1:1739:A:H2'   | 53:1:1740:G:O4'   | 2.21                     | 0.41              |
| 53:1:2391:G:O2'   | 53:1:2392:A:H8    | 2.04                     | 0.41              |
| 53:1:2588:G:H2'   | 53:1:2589:A:H5'   | 2.02                     | 0.41              |
| 53:1:2673:G:H2'   | 53:1:2674:G:C8    | 2.56                     | 0.41              |
| 53:1:2705:A:H2'   | 53:1:2706:A:O4'   | 2.21                     | 0.41              |
| 53:1:2825:G:H2'   | 53:1:2826:A:H5'   | 2.03                     | 0.41              |
| 58:8:207:ILE:HG22 | 58:8:271:ALA:H    | 1.84                     | 0.41              |
| 58:8:373:LEU:O    | 58:8:389:VAL:HG23 | 2.21                     | 0.41              |
| 1:b:24:HIS:HB3    | 1:b:81:GLU:OE1    | 2.21                     | 0.41              |
| 2:c:77:ARG:HH21   | 2:c:77:ARG:HG3    | 1.86                     | 0.41              |
| 3:d:128:ALA:HA    | 3:d:129:PRO:HD3   | 1.93                     | 0.41              |
| 5:f:28:LYS:HE2    | 5:f:28:LYS:HB3    | 1.90                     | 0.41              |
| 6:g:69:ALA:HA     | 6:g:72:ILE:HG13   | 2.03                     | 0.41              |
| 7:h:61:ARG:HD2    | 53:1:1046:A:O5'   | 2.21                     | 0.41              |
| 8:i:79:LEU:HA     | 8:i:82:ALA:HB3    | 2.03                     | 0.41              |
| 15:p:95:LYS:HD2   | 15:p:97:TYR:HE2   | 1.86                     | 0.41              |
| 16:q:18:LYS:HD3   | 16:q:18:LYS:C     | 2.45                     | 0.41              |
| 16:q:54:ARG:NH2   | 53:1:977:G:H5'    | 2.36                     | 0.41              |
| 21:v:64:VAL:HG22  | 21:v:69:GLU:HG2   | 2.01                     | 0.41              |
| 25:z:14:GLY:O     | 25:z:15:ARG:HD3   | 2.21                     | 0.41              |
| 32:H:181:ILE:HD12 | 32:H:181:ILE:N    | 2.35                     | 0.41              |
| 41:Q:32:VAL:HB    | 41:Q:55:ARG:HB3   | 2.02                     | 0.41              |
| 45:U:47:GLU:HG2   | 45:U:48:GLU:HG2   | 2.03                     | 0.41              |
| 51:a:5:THR:CG2    | 51:a:8:MET:HE3    | 2.49                     | 0.41              |
| 51:a:38:PHE:HD1   | 53:1:2127:G:H4'   | 1.84                     | 0.41              |
| 52:3:90:C:H2'     | 52:3:91:U:C5      | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:3:1005:A:H2'   | 52:3:1006:G:C5'   | 2.51                     | 0.41              |
| 52:3:1386:G:H2'   | 52:3:1387:G:C8    | 2.55                     | 0.41              |
| 53:1:1408:G:H2'   | 53:1:1409:U:O4'   | 2.21                     | 0.41              |
| 53:1:1655:A:H2'   | 53:1:1656:C:O4'   | 2.21                     | 0.41              |
| 53:1:1906:G:H2'   | 53:1:1907:G:C5'   | 2.33                     | 0.41              |
| 53:1:2271:G:H2'   | 53:1:2272:U:C6    | 2.55                     | 0.41              |
| 53:1:2751:G:O2'   | 53:1:2752:C:H5'   | 2.20                     | 0.41              |
| 7:h:59:LEU:HG     | 7:h:61:ARG:H      | 1.87                     | 0.40              |
| 7:h:94:ARG:HD3    | 7:h:94:ARG:N      | 2.35                     | 0.40              |
| 11:l:111:ILE:HD11 | 53:1:636:G:C5     | 2.56                     | 0.40              |
| 15:p:6:GLN:O      | 15:p:10:GLU:HG2   | 2.20                     | 0.40              |
| 15:p:90:ALA:HB2   | 15:p:112:ARG:HD3  | 2.03                     | 0.40              |
| 19:t:64:LYS:HA    | 19:t:64:LYS:HD3   | 1.86                     | 0.40              |
| 23:x:37:PHE:HE2   | 23:x:50:VAL:HG11  | 1.86                     | 0.40              |
| 26:B:24:VAL:HG23  | 26:B:25:THR:H     | 1.86                     | 0.40              |
| 30:F:24:ARG:HG2   | 30:F:36:ARG:CG    | 2.51                     | 0.40              |
| 31:G:105:THR:HG21 | 52:3:1072:G:N2    | 2.36                     | 0.40              |
| 32:H:24:ASN:HB2   | 32:H:27:GLU:OE1   | 2.21                     | 0.40              |
| 35:K:25:TYR:O     | 35:K:29:ILE:HG13  | 2.21                     | 0.40              |
| 37:M:44:PHE:CB    | 37:M:45:ILE:HD12  | 2.48                     | 0.40              |
| 38:N:114:LYS:HB2  | 38:N:117:LEU:HB2  | 2.03                     | 0.40              |
| 45:U:39:PHE:CZ    | 45:U:41:PRO:HB3   | 2.56                     | 0.40              |
| 48:X:30:LEU:HB2   | 48:X:48:ILE:HG23  | 2.03                     | 0.40              |
| 52:3:1075:U:H2'   | 52:3:1076:U:C6    | 2.55                     | 0.40              |
| 52:3:1094:G:N3    | 52:3:1094:G:H2'   | 2.35                     | 0.40              |
| 52:3:1157:A:H4'   | 52:3:1158:C:O5'   | 2.21                     | 0.40              |
| 53:1:139:U:H5'    | 53:1:140:C:OP1    | 2.21                     | 0.40              |
| 53:1:162:U:C2'    | 53:1:163:C:H5'    | 2.51                     | 0.40              |
| 53:1:976:G:H2'    | 53:1:977:G:C8     | 2.55                     | 0.40              |
| 53:1:1105:U:H2'   | 53:1:1106:G:C5'   | 2.51                     | 0.40              |
| 53:1:1609:A:H1'   | 53:1:1616:A:O4'   | 2.20                     | 0.40              |
| 53:1:1998:A:H2'   | 53:1:1999:C:C6    | 2.56                     | 0.40              |
| 58:8:9:THR:HG23   | 58:8:10:LYS:HG2   | 2.03                     | 0.40              |
| 58:8:211:PHE:HA   | 58:8:235:GLY:HA3  | 2.04                     | 0.40              |
| 7:h:91:ALA:O      | 7:h:92:ALA:HB3    | 2.22                     | 0.40              |
| 8:i:74:PRO:O      | 8:i:77:VAL:HG22   | 2.21                     | 0.40              |
| 11:l:90:VAL:HG13  | 11:l:95:LEU:HD21  | 2.02                     | 0.40              |
| 12:m:41:LEU:HD11  | 12:m:126:ILE:HD13 | 2.03                     | 0.40              |
| 17:r:27:ILE:HG22  | 17:r:28:ALA:N     | 2.36                     | 0.40              |
| 31:G:94:ARG:HH22  | 52:3:1100:C:H3'   | 1.85                     | 0.40              |
| 32:H:187:GLU:HG3  | 32:H:189:HIS:HE1  | 1.85                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:I:16:THR:HG22  | 33:I:17:ASP:H     | 1.86                     | 0.40              |
| 33:I:49:ASP:O     | 33:I:52:VAL:HG22  | 2.20                     | 0.40              |
| 33:I:143:SER:OG   | 33:I:144:ILE:N    | 2.51                     | 0.40              |
| 38:N:105:ARG:NE   | 52:3:1117:A:O3'   | 2.49                     | 0.40              |
| 41:Q:20:VAL:HG21  | 52:3:553:A:H5''   | 2.03                     | 0.40              |
| 44:T:44:GLU:O     | 44:T:45:HIS:HB2   | 2.21                     | 0.40              |
| 44:T:88:ARG:H     | 44:T:88:ARG:CD    | 2.35                     | 0.40              |
| 47:W:52:ARG:HH21  | 52:3:664:G:H5'    | 1.86                     | 0.40              |
| 51:a:8:MET:CE     | 53:1:2174:C:H5''  | 2.52                     | 0.40              |
| 52:3:389:A:N3     | 52:3:389:A:H2'    | 2.36                     | 0.40              |
| 52:3:494:G:O2'    | 52:3:496:A:H1'    | 2.21                     | 0.40              |
| 52:3:502:A:H2'    | 52:3:503:C:O4'    | 2.21                     | 0.40              |
| 52:3:679:C:H2'    | 52:3:680:C:C6     | 2.57                     | 0.40              |
| 52:3:886:G:H2'    | 52:3:887:G:O4'    | 2.21                     | 0.40              |
| 53:1:248:G:N3     | 53:1:2431:U:H4'   | 2.36                     | 0.40              |
| 53:1:292:U:H2'    | 53:1:293:U:C6     | 2.56                     | 0.40              |
| 53:1:596:U:H2'    | 53:1:597:G:H8     | 1.86                     | 0.40              |
| 53:1:2364:C:H2'   | 53:1:2365:G:O4'   | 2.20                     | 0.40              |
| 54:2:48:U:H2'     | 54:2:49:C:H6      | 1.86                     | 0.40              |
| 55:6:34:C:O2      | 55:6:34:C:C2'     | 2.68                     | 0.40              |
| 1:b:157:ALA:HB1   | 1:b:196:ASN:O     | 2.21                     | 0.40              |
| 6:g:5:LEU:HD12    | 6:g:5:LEU:N       | 2.36                     | 0.40              |
| 6:g:46:PHE:HB3    | 6:g:50:ARG:HH21   | 1.85                     | 0.40              |
| 8:i:139:VAL:O     | 8:i:139:VAL:HG23  | 2.21                     | 0.40              |
| 10:k:76:VAL:H     | 15:p:72:VAL:CG1   | 2.33                     | 0.40              |
| 11:l:85:VAL:O     | 11:l:86:GLU:HG2   | 2.21                     | 0.40              |
| 12:m:123:LYS:NZ   | 53:1:2483:C:H42   | 2.19                     | 0.40              |
| 13:n:51:LEU:HD11  | 13:n:70:THR:CG2   | 2.48                     | 0.40              |
| 15:p:38:ARG:NH1   | 52:3:345:C:H5'    | 2.37                     | 0.40              |
| 17:r:51:VAL:CG2   | 17:r:52:PRO:HD2   | 2.51                     | 0.40              |
| 18:s:41:LYS:CD    | 53:1:2009:A:H5''  | 2.51                     | 0.40              |
| 31:G:114:LYS:HA   | 31:G:117:GLU:HG2  | 2.03                     | 0.40              |
| 31:G:209:VAL:O    | 31:G:213:LEU:HD13 | 2.22                     | 0.40              |
| 33:I:85:THR:H     | 34:J:102:THR:HG21 | 1.86                     | 0.40              |
| 36:L:30:MET:SD    | 52:3:1373:G:H4'   | 2.61                     | 0.40              |
| 40:P:85:VAL:CG2   | 40:P:92:ARG:HD2   | 2.51                     | 0.40              |
| 41:Q:24:GLU:OE2   | 41:Q:24:GLU:N     | 2.50                     | 0.40              |
| 41:Q:106:VAL:HG22 | 41:Q:116:TYR:HB3  | 2.04                     | 0.40              |
| 45:U:36:VAL:HG13  | 45:U:53:ASP:HB3   | 2.03                     | 0.40              |
| 45:U:54:LEU:HA    | 45:U:57:ILE:HD12  | 2.03                     | 0.40              |
| 52:3:346:G:C2'    | 52:3:347:G:H5'    | 2.51                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:3:545:C:O2'    | 52:3:549:C:H5''   | 2.22                     | 0.40              |
| 52:3:766:A:H2'    | 52:3:767:A:O4'    | 2.21                     | 0.40              |
| 52:3:1245:C:H2'   | 52:3:1246:A:C8    | 2.56                     | 0.40              |
| 53:1:162:U:H2'    | 53:1:163:C:H5'    | 2.03                     | 0.40              |
| 53:1:1863:G:H4'   | 53:1:2411:A:H4'   | 2.03                     | 0.40              |
| 53:1:2093:G:N7    | 53:1:2225:A:H2'   | 2.37                     | 0.40              |
| 53:1:2286:G:C4'   | 53:1:2287:A:O4'   | 2.68                     | 0.40              |
| 53:1:2372:U:H2'   | 53:1:2373:G:C8    | 2.57                     | 0.40              |
| 53:1:2388:A:H5'   | 53:1:2389:G:OP2   | 2.21                     | 0.40              |
| 53:1:2628:C:O2'   | 53:1:2781:A:H2'   | 2.20                     | 0.40              |
| 54:2:30:C:H2'     | 54:2:31:C:H5'     | 2.04                     | 0.40              |
| 3:d:119:ILE:HB    | 3:d:187:VAL:HG12  | 2.04                     | 0.40              |
| 8:i:124:MET:O     | 8:i:127:SER:OG    | 2.34                     | 0.40              |
| 12:m:6:ARG:NH2    | 53:1:870:U:OP1    | 2.55                     | 0.40              |
| 12:m:41:LEU:N     | 12:m:41:LEU:HD12  | 2.36                     | 0.40              |
| 14:o:15:ARG:NH2   | 54:2:8:C:H5''     | 2.37                     | 0.40              |
| 24:y:24:GLU:O     | 24:y:28:LEU:N     | 2.54                     | 0.40              |
| 30:F:11:CYS:HB3   | 30:F:33:HIS:HE1   | 1.85                     | 0.40              |
| 31:G:7:ASP:HA     | 31:G:10:LYS:HB3   | 2.04                     | 0.40              |
| 32:H:170:GLY:O    | 52:3:1106:G:H4'   | 2.22                     | 0.40              |
| 32:H:179:ALA:HB3  | 32:H:181:ILE:HD11 | 2.03                     | 0.40              |
| 34:J:113:VAL:HG13 | 34:J:114:LEU:HD12 | 2.02                     | 0.40              |
| 36:L:91:ARG:O     | 36:L:95:ARG:N     | 2.52                     | 0.40              |
| 38:N:78:ILE:O     | 38:N:82:ILE:HG12  | 2.22                     | 0.40              |
| 43:S:63:CYS:SG    | 43:S:64:ARG:N     | 2.95                     | 0.40              |
| 49:Y:76:ALA:O     | 49:Y:79:THR:OG1   | 2.31                     | 0.40              |
| 51:a:6:LYS:HG3    | 51:a:7:ARG:H      | 1.87                     | 0.40              |
| 52:3:309:A:H2'    | 52:3:310:G:H8     | 1.86                     | 0.40              |
| 52:3:346:G:H2'    | 52:3:347:G:H5'    | 2.03                     | 0.40              |
| 53:1:1956:U:C2'   | 53:1:1957:C:H5'   | 2.51                     | 0.40              |
| 6:g:24:GLY:HA3    | 53:1:2093:G:O5'   | 2.22                     | 0.40              |
| 7:h:112:ALA:O     | 7:h:113:PHE:C     | 2.64                     | 0.40              |
| 9:j:42:ALA:O      | 16:q:99:VAL:HG12  | 2.21                     | 0.40              |
| 11:l:132:ARG:HH12 | 11:l:142:ILE:HG21 | 1.85                     | 0.40              |
| 13:n:79:LEU:C     | 13:n:81:ASN:H     | 2.30                     | 0.40              |
| 23:x:30:PRO:HG2   | 23:x:32:LEU:HG    | 2.03                     | 0.40              |
| 24:y:40:SER:O     | 24:y:43:LEU:HG    | 2.22                     | 0.40              |
| 26:B:9:ARG:NH2    | 26:B:9:ARG:HG3    | 2.37                     | 0.40              |
| 33:I:14:GLU:HG2   | 33:I:55:ARG:HH21  | 1.85                     | 0.40              |
| 34:J:73:VAL:O     | 34:J:73:VAL:HG13  | 2.20                     | 0.40              |
| 39:O:53:ILE:HG12  | 52:3:1060:U:H5''  | 2.02                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 44:T:44:GLU:HG2  | 44:T:45:HIS:HD2  | 1.86                     | 0.40              |
| 49:Y:2:ASN:HB3   | 52:3:332:G:OP2   | 2.21                     | 0.40              |
| 50:Z:35:GLU:O    | 50:Z:36:PHE:HB2  | 2.20                     | 0.40              |
| 51:a:168:ASN:ND2 | 53:1:2179:C:H5'  | 2.34                     | 0.40              |
| 52:3:782:A:H2'   | 52:3:783:C:H5'   | 2.03                     | 0.40              |
| 53:1:63:A:H2'    | 53:1:64:A:C8     | 2.56                     | 0.40              |
| 53:1:1491:G:H2'  | 53:1:1492:G:H8   | 1.85                     | 0.40              |
| 53:1:1535:A:H3'  | 53:1:1536:C:H5'  | 2.04                     | 0.40              |
| 53:1:1925:C:O2'  | 53:1:1926:U:H5'  | 2.22                     | 0.40              |
| 53:1:2008:C:H2'  | 53:1:2009:A:C8   | 2.57                     | 0.40              |
| 53:1:2120:G:H2'  | 53:1:2121:G:C8   | 2.54                     | 0.40              |
| 53:1:2294:G:H2'  | 53:1:2295:C:H6   | 1.87                     | 0.40              |
| 53:1:2654:A:N1   | 53:1:2665:A:H5'' | 2.36                     | 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%) | 233 (87%) | 32 (12%) | 4 (2%)   | 8           | 37  |
| 2   | c     | 207/209 (99%) | 181 (87%) | 24 (12%) | 2 (1%)   | 12          | 45  |
| 3   | d     | 199/201 (99%) | 176 (88%) | 21 (11%) | 2 (1%)   | 12          | 45  |
| 4   | e     | 175/177 (99%) | 153 (87%) | 22 (13%) | 0        | 100         | 100 |
| 5   | f     | 174/176 (99%) | 156 (90%) | 17 (10%) | 1 (1%)   | 21          | 54  |
| 6   | g     | 147/149 (99%) | 129 (88%) | 17 (12%) | 1 (1%)   | 18          | 51  |
| 7   | h     | 129/131 (98%) | 102 (79%) | 20 (16%) | 7 (5%)   | 1           | 14  |
| 8   | i     | 139/141 (99%) | 121 (87%) | 16 (12%) | 2 (1%)   | 9           | 38  |
| 9   | j     | 140/142 (99%) | 133 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 10  | k     | 120/122 (98%) | 103 (86%) | 14 (12%) | 3 (2%)   | 4           | 28  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 11  | l     | 141/143 (99%) | 119 (84%) | 20 (14%) | 2 (1%)   | 9           | 38  |
| 12  | m     | 134/136 (98%) | 120 (90%) | 11 (8%)  | 3 (2%)   | 5           | 30  |
| 13  | n     | 118/120 (98%) | 102 (86%) | 13 (11%) | 3 (2%)   | 4           | 28  |
| 14  | o     | 114/116 (98%) | 103 (90%) | 9 (8%)   | 2 (2%)   | 6           | 34  |
| 15  | p     | 112/114 (98%) | 102 (91%) | 9 (8%)   | 1 (1%)   | 14          | 46  |
| 16  | q     | 115/117 (98%) | 108 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 17  | r     | 101/103 (98%) | 81 (80%)  | 18 (18%) | 2 (2%)   | 6           | 32  |
| 18  | s     | 108/110 (98%) | 92 (85%)  | 13 (12%) | 3 (3%)   | 4           | 26  |
| 19  | t     | 91/93 (98%)   | 79 (87%)  | 12 (13%) | 0        | 100         | 100 |
| 20  | u     | 100/102 (98%) | 84 (84%)  | 16 (16%) | 0        | 100         | 100 |
| 21  | v     | 92/94 (98%)   | 85 (92%)  | 7 (8%)   | 0        | 100         | 100 |
| 22  | w     | 73/75 (97%)   | 65 (89%)  | 7 (10%)  | 1 (1%)   | 9           | 38  |
| 23  | x     | 75/77 (97%)   | 69 (92%)  | 6 (8%)   | 0        | 100         | 100 |
| 24  | y     | 61/63 (97%)   | 58 (95%)  | 2 (3%)   | 1 (2%)   | 7           | 36  |
| 25  | z     | 56/58 (97%)   | 52 (93%)  | 4 (7%)   | 0        | 100         | 100 |
| 26  | B     | 54/56 (96%)   | 51 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 27  | C     | 48/50 (96%)   | 47 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 28  | D     | 44/46 (96%)   | 40 (91%)  | 4 (9%)   | 0        | 100         | 100 |
| 29  | E     | 62/64 (97%)   | 55 (89%)  | 6 (10%)  | 1 (2%)   | 7           | 36  |
| 30  | F     | 36/38 (95%)   | 30 (83%)  | 5 (14%)  | 1 (3%)   | 4           | 26  |
| 31  | G     | 223/225 (99%) | 207 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 32  | H     | 204/206 (99%) | 192 (94%) | 11 (5%)  | 1 (0%)   | 24          | 57  |
| 33  | I     | 203/205 (99%) | 183 (90%) | 17 (8%)  | 3 (2%)   | 8           | 37  |
| 34  | J     | 155/157 (99%) | 130 (84%) | 22 (14%) | 3 (2%)   | 6           | 33  |
| 35  | K     | 98/100 (98%)  | 79 (81%)  | 14 (14%) | 5 (5%)   | 1           | 15  |
| 36  | L     | 149/151 (99%) | 134 (90%) | 15 (10%) | 0        | 100         | 100 |
| 37  | M     | 127/129 (98%) | 108 (85%) | 16 (13%) | 3 (2%)   | 4           | 29  |
| 38  | N     | 125/127 (98%) | 100 (80%) | 20 (16%) | 5 (4%)   | 2           | 20  |
| 39  | O     | 96/98 (98%)   | 77 (80%)  | 15 (16%) | 4 (4%)   | 2           | 19  |
| 40  | P     | 114/116 (98%) | 97 (85%)  | 14 (12%) | 3 (3%)   | 4           | 27  |
| 41  | Q     | 121/123 (98%) | 94 (78%)  | 14 (12%) | 13 (11%) | 0           | 5   |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 42  | R     | 112/114 (98%)   | 95 (85%)   | 13 (12%)  | 4 (4%)   | 2           | 22  |
| 43  | S     | 98/100 (98%)    | 83 (85%)   | 15 (15%)  | 0        | 100         | 100 |
| 44  | T     | 86/88 (98%)     | 80 (93%)   | 5 (6%)    | 1 (1%)   | 10          | 41  |
| 45  | U     | 80/82 (98%)     | 67 (84%)   | 10 (12%)  | 3 (4%)   | 2           | 21  |
| 46  | V     | 78/80 (98%)     | 65 (83%)   | 11 (14%)  | 2 (3%)   | 4           | 27  |
| 47  | W     | 63/65 (97%)     | 57 (90%)   | 5 (8%)    | 1 (2%)   | 7           | 36  |
| 48  | X     | 77/79 (98%)     | 61 (79%)   | 15 (20%)  | 1 (1%)   | 9           | 39  |
| 49  | Y     | 83/85 (98%)     | 78 (94%)   | 5 (6%)    | 0        | 100         | 100 |
| 50  | Z     | 63/65 (97%)     | 41 (65%)   | 16 (25%)  | 6 (10%)  | 0           | 6   |
| 51  | a     | 130/223 (58%)   | 125 (96%)  | 5 (4%)    | 0        | 100         | 100 |
| 58  | 8     | 390/400 (98%)   | 356 (91%)  | 32 (8%)   | 2 (0%)   | 24          | 57  |
| All | All   | 6309/6512 (97%) | 5538 (88%) | 669 (11%) | 102 (2%) | 10          | 36  |

All (102) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 232 | GLY  |
| 2   | c     | 86  | GLU  |
| 3   | d     | 83  | VAL  |
| 7   | h     | 118 | ILE  |
| 17  | r     | 54  | VAL  |
| 24  | y     | 24  | GLU  |
| 29  | E     | 31  | ILE  |
| 30  | F     | 37  | GLN  |
| 34  | J     | 93  | VAL  |
| 34  | J     | 122 | VAL  |
| 35  | K     | 92  | THR  |
| 37  | M     | 47  | ASP  |
| 38  | N     | 90  | ASP  |
| 38  | N     | 125 | GLN  |
| 40  | P     | 125 | LYS  |
| 41  | Q     | 101 | LEU  |
| 42  | R     | 65  | GLU  |
| 45  | U     | 79  | ASN  |
| 46  | V     | 49  | ASN  |
| 50  | Z     | 8   | ASN  |
| 50  | Z     | 14  | ALA  |
| 5   | f     | 175 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | g     | 9   | VAL  |
| 7   | h     | 108 | VAL  |
| 10  | k     | 89  | ASN  |
| 13  | n     | 14  | SER  |
| 18  | s     | 40  | ASN  |
| 35  | K     | 56  | LYS  |
| 37  | M     | 88  | LYS  |
| 38  | N     | 57  | VAL  |
| 38  | N     | 71  | ILE  |
| 39  | O     | 58  | ASN  |
| 40  | P     | 89  | GLY  |
| 41  | Q     | 3   | VAL  |
| 41  | Q     | 24  | GLU  |
| 41  | Q     | 33  | CYS  |
| 41  | Q     | 35  | ARG  |
| 41  | Q     | 88  | ASP  |
| 42  | R     | 4   | ALA  |
| 46  | V     | 17  | GLU  |
| 47  | W     | 13  | THR  |
| 58  | 8     | 250 | GLU  |
| 7   | h     | 58  | THR  |
| 7   | h     | 80  | THR  |
| 12  | m     | 58  | LYS  |
| 12  | m     | 59  | ARG  |
| 12  | m     | 69  | PRO  |
| 14  | o     | 34  | HIS  |
| 15  | p     | 113 | LEU  |
| 32  | H     | 156 | LEU  |
| 33  | I     | 4   | LEU  |
| 33  | I     | 28  | ASP  |
| 34  | J     | 11  | GLN  |
| 39  | O     | 37  | ARG  |
| 41  | Q     | 102 | ASP  |
| 42  | R     | 7   | ASN  |
| 45  | U     | 46  | LYS  |
| 45  | U     | 47  | GLU  |
| 50  | Z     | 12  | ASP  |
| 50  | Z     | 34  | ARG  |
| 1   | b     | 175 | LEU  |
| 7   | h     | 81  | LEU  |
| 8   | i     | 11  | GLN  |
| 11  | l     | 29  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | n     | 107 | ASN  |
| 13  | n     | 117 | ASP  |
| 17  | r     | 44  | GLY  |
| 18  | s     | 11  | ARG  |
| 35  | K     | 86  | ARG  |
| 38  | N     | 100 | ALA  |
| 39  | O     | 56  | HIS  |
| 40  | P     | 88  | PRO  |
| 41  | Q     | 2   | THR  |
| 48  | X     | 76  | THR  |
| 50  | Z     | 24  | LYS  |
| 50  | Z     | 66  | ARG  |
| 58  | 8     | 4   | GLU  |
| 2   | c     | 148 | GLN  |
| 3   | d     | 80  | SER  |
| 10  | k     | 110 | GLU  |
| 14  | o     | 116 | GLN  |
| 18  | s     | 63  | GLY  |
| 22  | w     | 80  | ALA  |
| 35  | K     | 95  | ALA  |
| 39  | O     | 42  | LEU  |
| 41  | Q     | 117 | GLY  |
| 44  | T     | 2   | LEU  |
| 33  | I     | 166 | LYS  |
| 35  | K     | 42  | TRP  |
| 37  | M     | 56  | PRO  |
| 41  | Q     | 75  | GLU  |
| 1   | b     | 125 | PRO  |
| 10  | k     | 72  | PRO  |
| 7   | h     | 119 | PRO  |
| 11  | l     | 88  | GLY  |
| 41  | Q     | 78  | VAL  |
| 42  | R     | 6   | ILE  |
| 1   | b     | 106 | PRO  |
| 7   | h     | 79  | PRO  |
| 41  | Q     | 41  | PRO  |
| 41  | Q     | 43  | LYS  |
| 8   | i     | 12  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | b     | 216/216 (100%) | 215 (100%) | 1 (0%)   | 81          | 80  |
| 2   | c     | 164/164 (100%) | 164 (100%) | 0        | 100         | 100 |
| 3   | d     | 165/165 (100%) | 164 (99%)  | 1 (1%)   | 78          | 79  |
| 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%) | 115 (99%)  | 1 (1%)   | 70          | 76  |
| 10  | k     | 103/103 (100%) | 101 (98%)  | 2 (2%)   | 50          | 67  |
| 11  | l     | 102/102 (100%) | 102 (100%) | 0        | 100         | 100 |
| 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%)   | 86 (100%)  | 0        | 100         | 100 |
| 15  | p     | 99/99 (100%)   | 99 (100%)  | 0        | 100         | 100 |
| 16  | q     | 89/89 (100%)   | 88 (99%)   | 1 (1%)   | 65          | 74  |
| 17  | r     | 84/84 (100%)   | 83 (99%)   | 1 (1%)   | 63          | 73  |
| 18  | s     | 93/93 (100%)   | 92 (99%)   | 1 (1%)   | 65          | 74  |
| 19  | t     | 80/80 (100%)   | 79 (99%)   | 1 (1%)   | 61          | 72  |
| 20  | u     | 83/83 (100%)   | 83 (100%)  | 0        | 100         | 100 |
| 21  | v     | 78/78 (100%)   | 77 (99%)   | 1 (1%)   | 61          | 72  |
| 22  | w     | 57/57 (100%)   | 57 (100%)  | 0        | 100         | 100 |
| 23  | x     | 67/67 (100%)   | 67 (100%)  | 0        | 100         | 100 |
| 24  | y     | 55/55 (100%)   | 55 (100%)  | 0        | 100         | 100 |
| 25  | z     | 48/48 (100%)   | 48 (100%)  | 0        | 100         | 100 |
| 26  | B     | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 27  | C     | 45/45 (100%)    | 44 (98%)    | 1 (2%)   | 45          | 65  |
| 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%)    | 34 (100%)   | 0        | 100         | 100 |
| 31  | G     | 186/186 (100%)  | 184 (99%)   | 2 (1%)   | 65          | 74  |
| 32  | H     | 170/170 (100%)  | 170 (100%)  | 0        | 100         | 100 |
| 33  | I     | 172/172 (100%)  | 172 (100%)  | 0        | 100         | 100 |
| 34  | J     | 119/119 (100%)  | 119 (100%)  | 0        | 100         | 100 |
| 35  | K     | 87/87 (100%)    | 87 (100%)   | 0        | 100         | 100 |
| 36  | L     | 124/124 (100%)  | 124 (100%)  | 0        | 100         | 100 |
| 37  | M     | 104/104 (100%)  | 104 (100%)  | 0        | 100         | 100 |
| 38  | N     | 105/105 (100%)  | 105 (100%)  | 0        | 100         | 100 |
| 39  | O     | 86/86 (100%)    | 84 (98%)    | 2 (2%)   | 44          | 64  |
| 40  | P     | 89/89 (100%)    | 89 (100%)   | 0        | 100         | 100 |
| 41  | Q     | 103/103 (100%)  | 103 (100%)  | 0        | 100         | 100 |
| 42  | R     | 92/92 (100%)    | 90 (98%)    | 2 (2%)   | 45          | 65  |
| 43  | S     | 83/83 (100%)    | 83 (100%)   | 0        | 100         | 100 |
| 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%)    | 74 (100%)   | 0        | 100         | 100 |
| 47  | W     | 56/56 (100%)    | 56 (100%)   | 0        | 100         | 100 |
| 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%)    | 54 (98%)    | 1 (2%)   | 51          | 68  |
| 51  | a     | 110/174 (63%)   | 110 (100%)  | 0        | 100         | 100 |
| 58  | 8     | 324/332 (98%)   | 324 (100%)  | 0        | 100         | 100 |
| All | All   | 5232/5304 (99%) | 5209 (100%) | 23 (0%)  | 81          | 81  |

All (23) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 227 | VAL  |
| 3   | d     | 176 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | h     | 118 | ILE  |
| 7   | h     | 119 | PRO  |
| 8   | i     | 12  | VAL  |
| 9   | j     | 49  | ASP  |
| 10  | k     | 37  | ASP  |
| 10  | k     | 88  | ASN  |
| 12  | m     | 25  | ASP  |
| 16  | q     | 5   | ARG  |
| 17  | r     | 54  | VAL  |
| 18  | s     | 77  | ASP  |
| 19  | t     | 32  | LEU  |
| 21  | v     | 12  | GLN  |
| 27  | C     | 46  | VAL  |
| 31  | G     | 9   | LEU  |
| 31  | G     | 191 | ASP  |
| 39  | O     | 69  | THR  |
| 39  | O     | 89  | ARG  |
| 42  | R     | 101 | THR  |
| 42  | R     | 104 | ASN  |
| 45  | U     | 74  | LEU  |
| 50  | Z     | 40  | PRO  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 44  | ASN  |
| 1   | b     | 45  | ASN  |
| 1   | b     | 89  | ASN  |
| 1   | b     | 127 | ASN  |
| 1   | b     | 133 | ASN  |
| 2   | c     | 32  | ASN  |
| 2   | c     | 49  | GLN  |
| 3   | d     | 46  | GLN  |
| 3   | d     | 97  | ASN  |
| 4   | e     | 51  | ASN  |
| 5   | f     | 63  | GLN  |
| 5   | f     | 87  | GLN  |
| 6   | g     | 2   | GLN  |
| 6   | g     | 28  | ASN  |
| 6   | g     | 66  | ASN  |
| 6   | g     | 73  | ASN  |
| 6   | g     | 133 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | i     | 30  | GLN  |
| 9   | j     | 40  | HIS  |
| 9   | j     | 58  | ASN  |
| 9   | j     | 135 | GLN  |
| 10  | k     | 5   | GLN  |
| 11  | l     | 38  | GLN  |
| 11  | l     | 54  | GLN  |
| 12  | m     | 3   | GLN  |
| 13  | n     | 9   | GLN  |
| 13  | n     | 62  | ASN  |
| 13  | n     | 81  | ASN  |
| 14  | o     | 19  | GLN  |
| 14  | o     | 98  | GLN  |
| 14  | o     | 100 | HIS  |
| 14  | o     | 104 | GLN  |
| 15  | p     | 11  | GLN  |
| 15  | p     | 40  | GLN  |
| 15  | p     | 76  | HIS  |
| 17  | r     | 43  | ASN  |
| 17  | r     | 82  | HIS  |
| 19  | t     | 15  | HIS  |
| 19  | t     | 59  | ASN  |
| 19  | t     | 70  | HIS  |
| 19  | t     | 92  | ASN  |
| 20  | u     | 39  | ASN  |
| 20  | u     | 52  | ASN  |
| 20  | u     | 68  | ASN  |
| 20  | u     | 73  | ASN  |
| 21  | v     | 49  | ASN  |
| 21  | v     | 78  | GLN  |
| 24  | y     | 41  | HIS  |
| 25  | z     | 8   | GLN  |
| 27  | C     | 18  | HIS  |
| 27  | C     | 25  | ASN  |
| 28  | D     | 6   | GLN  |
| 30  | F     | 35  | GLN  |
| 31  | G     | 17  | HIS  |
| 31  | G     | 41  | ASN  |
| 31  | G     | 108 | GLN  |
| 31  | G     | 119 | GLN  |
| 31  | G     | 176 | ASN  |
| 31  | G     | 177 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | G     | 202 | ASN  |
| 32  | H     | 2   | GLN  |
| 32  | H     | 139 | ASN  |
| 32  | H     | 184 | ASN  |
| 32  | H     | 189 | HIS  |
| 33  | I     | 88  | ASN  |
| 33  | I     | 130 | ASN  |
| 33  | I     | 135 | GLN  |
| 33  | I     | 163 | GLN  |
| 33  | I     | 197 | HIS  |
| 34  | J     | 72  | ASN  |
| 35  | K     | 3   | HIS  |
| 35  | K     | 17  | GLN  |
| 35  | K     | 46  | GLN  |
| 35  | K     | 52  | ASN  |
| 35  | K     | 55  | HIS  |
| 35  | K     | 68  | GLN  |
| 36  | L     | 27  | ASN  |
| 36  | L     | 121 | ASN  |
| 38  | N     | 30  | ASN  |
| 39  | O     | 58  | ASN  |
| 40  | P     | 14  | GLN  |
| 41  | Q     | 4   | ASN  |
| 41  | Q     | 45  | ASN  |
| 41  | Q     | 58  | ASN  |
| 43  | S     | 42  | ASN  |
| 44  | T     | 27  | GLN  |
| 44  | T     | 34  | GLN  |
| 44  | T     | 36  | ASN  |
| 44  | T     | 49  | HIS  |
| 45  | U     | 9   | HIS  |
| 45  | U     | 63  | GLN  |
| 46  | V     | 8   | GLN  |
| 46  | V     | 30  | HIS  |
| 46  | V     | 46  | HIS  |
| 47  | W     | 30  | ASN  |
| 47  | W     | 53  | GLN  |
| 48  | X     | 55  | GLN  |
| 48  | X     | 56  | HIS  |
| 49  | Y     | 12  | GLN  |
| 49  | Y     | 51  | ASN  |
| 49  | Y     | 60  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | Y     | 67  | HIS  |
| 49  | Y     | 69  | ASN  |
| 49  | Y     | 74  | HIS  |
| 49  | Y     | 77  | ASN  |
| 49  | Y     | 83  | ASN  |
| 50  | Z     | 55  | HIS  |
| 51  | a     | 57  | GLN  |
| 51  | a     | 67  | HIS  |
| 51  | a     | 160 | GLN  |
| 51  | a     | 168 | ASN  |
| 51  | a     | 172 | HIS  |
| 51  | a     | 203 | GLN  |
| 58  | 8     | 67  | HIS  |
| 58  | 8     | 98  | GLN  |
| 58  | 8     | 125 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 52  | 3     | 1538/1539 (99%) | 136 (8%)          | 5 (0%)          |
| 53  | 1     | 2902/2903 (99%) | 324 (11%)         | 10 (0%)         |
| 54  | 2     | 119/120 (99%)   | 12 (10%)          | 1 (0%)          |
| 55  | 5     | 76/77 (98%)     | 7 (9%)            | 0               |
| 55  | 6     | 76/77 (98%)     | 8 (10%)           | 0               |
| 56  | 4     | 17/18 (94%)     | 3 (17%)           | 0               |
| 57  | 7     | 75/76 (98%)     | 14 (18%)          | 0               |
| All | All   | 4803/4810 (99%) | 504 (10%)         | 16 (0%)         |

All (504) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | 3     | 6   | G    |
| 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     | 87  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | 3     | 95  | C    |
| 52  | 3     | 100 | G    |
| 52  | 3     | 144 | G    |
| 52  | 3     | 183 | C    |
| 52  | 3     | 184 | G    |
| 52  | 3     | 197 | A    |
| 52  | 3     | 210 | C    |
| 52  | 3     | 211 | G    |
| 52  | 3     | 226 | G    |
| 52  | 3     | 247 | G    |
| 52  | 3     | 251 | G    |
| 52  | 3     | 253 | A    |
| 52  | 3     | 266 | G    |
| 52  | 3     | 267 | C    |
| 52  | 3     | 281 | G    |
| 52  | 3     | 289 | G    |
| 52  | 3     | 345 | C    |
| 52  | 3     | 352 | C    |
| 52  | 3     | 355 | C    |
| 52  | 3     | 367 | U    |
| 52  | 3     | 372 | C    |
| 52  | 3     | 412 | A    |
| 52  | 3     | 413 | G    |
| 52  | 3     | 422 | C    |
| 52  | 3     | 429 | U    |
| 52  | 3     | 439 | U    |
| 52  | 3     | 467 | U    |
| 52  | 3     | 485 | U    |
| 52  | 3     | 486 | U    |
| 52  | 3     | 496 | A    |
| 52  | 3     | 518 | C    |
| 52  | 3     | 527 | G    |
| 52  | 3     | 531 | U    |
| 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    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 52  | 3     | 642  | A    |
| 52  | 3     | 665  | A    |
| 52  | 3     | 688  | G    |
| 52  | 3     | 703  | G    |
| 52  | 3     | 724  | G    |
| 52  | 3     | 755  | G    |
| 52  | 3     | 777  | A    |
| 52  | 3     | 805  | C    |
| 52  | 3     | 815  | A    |
| 52  | 3     | 817  | C    |
| 52  | 3     | 818  | G    |
| 52  | 3     | 819  | A    |
| 52  | 3     | 843  | U    |
| 52  | 3     | 844  | G    |
| 52  | 3     | 846  | G    |
| 52  | 3     | 871  | U    |
| 52  | 3     | 873  | A    |
| 52  | 3     | 902  | G    |
| 52  | 3     | 926  | G    |
| 52  | 3     | 934  | C    |
| 52  | 3     | 935  | A    |
| 52  | 3     | 960  | U    |
| 52  | 3     | 961  | U    |
| 52  | 3     | 966  | G    |
| 52  | 3     | 969  | A    |
| 52  | 3     | 975  | A    |
| 52  | 3     | 976  | G    |
| 52  | 3     | 977  | A    |
| 52  | 3     | 991  | U    |
| 52  | 3     | 992  | U    |
| 52  | 3     | 993  | G    |
| 52  | 3     | 994  | A    |
| 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     | 1053 | G    |
| 52  | 3     | 1094 | G    |
| 52  | 3     | 1101 | A    |
| 52  | 3     | 1137 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 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     | 1196 | A    |
| 52  | 3     | 1198 | G    |
| 52  | 3     | 1201 | A    |
| 52  | 3     | 1202 | U    |
| 52  | 3     | 1225 | A    |
| 52  | 3     | 1238 | A    |
| 52  | 3     | 1240 | U    |
| 52  | 3     | 1241 | G    |
| 52  | 3     | 1258 | G    |
| 52  | 3     | 1260 | G    |
| 52  | 3     | 1275 | A    |
| 52  | 3     | 1278 | G    |
| 52  | 3     | 1280 | A    |
| 52  | 3     | 1282 | C    |
| 52  | 3     | 1286 | U    |
| 52  | 3     | 1287 | A    |
| 52  | 3     | 1300 | G    |
| 52  | 3     | 1317 | C    |
| 52  | 3     | 1320 | C    |
| 52  | 3     | 1346 | A    |
| 52  | 3     | 1347 | G    |
| 52  | 3     | 1363 | A    |
| 52  | 3     | 1364 | U    |
| 52  | 3     | 1378 | C    |
| 52  | 3     | 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     | 1533 | C    |
| 52  | 3     | 1540 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 1     | 10  | A    |
| 53  | 1     | 12  | U    |
| 53  | 1     | 34  | U    |
| 53  | 1     | 35  | G    |
| 53  | 1     | 51  | G    |
| 53  | 1     | 63  | A    |
| 53  | 1     | 71  | A    |
| 53  | 1     | 74  | A    |
| 53  | 1     | 75  | G    |
| 53  | 1     | 102 | U    |
| 53  | 1     | 119 | A    |
| 53  | 1     | 120 | U    |
| 53  | 1     | 139 | U    |
| 53  | 1     | 140 | C    |
| 53  | 1     | 141 | G    |
| 53  | 1     | 142 | A    |
| 53  | 1     | 162 | U    |
| 53  | 1     | 163 | C    |
| 53  | 1     | 181 | A    |
| 53  | 1     | 196 | A    |
| 53  | 1     | 216 | A    |
| 53  | 1     | 221 | A    |
| 53  | 1     | 222 | A    |
| 53  | 1     | 248 | G    |
| 53  | 1     | 249 | C    |
| 53  | 1     | 255 | A    |
| 53  | 1     | 265 | A    |
| 53  | 1     | 266 | G    |
| 53  | 1     | 276 | U    |
| 53  | 1     | 281 | C    |
| 53  | 1     | 294 | A    |
| 53  | 1     | 301 | G    |
| 53  | 1     | 311 | A    |
| 53  | 1     | 323 | C    |
| 53  | 1     | 324 | A    |
| 53  | 1     | 329 | G    |
| 53  | 1     | 330 | A    |
| 53  | 1     | 371 | A    |
| 53  | 1     | 372 | G    |
| 53  | 1     | 386 | G    |
| 53  | 1     | 387 | U    |
| 53  | 1     | 404 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 1     | 406 | G    |
| 53  | 1     | 411 | G    |
| 53  | 1     | 422 | A    |
| 53  | 1     | 424 | G    |
| 53  | 1     | 443 | A    |
| 53  | 1     | 444 | C    |
| 53  | 1     | 451 | U    |
| 53  | 1     | 457 | A    |
| 53  | 1     | 458 | G    |
| 53  | 1     | 481 | G    |
| 53  | 1     | 491 | G    |
| 53  | 1     | 504 | A    |
| 53  | 1     | 505 | A    |
| 53  | 1     | 529 | A    |
| 53  | 1     | 530 | G    |
| 53  | 1     | 531 | C    |
| 53  | 1     | 532 | A    |
| 53  | 1     | 543 | G    |
| 53  | 1     | 563 | A    |
| 53  | 1     | 572 | A    |
| 53  | 1     | 573 | U    |
| 53  | 1     | 574 | A    |
| 53  | 1     | 588 | U    |
| 53  | 1     | 603 | A    |
| 53  | 1     | 616 | A    |
| 53  | 1     | 627 | A    |
| 53  | 1     | 628 | G    |
| 53  | 1     | 637 | A    |
| 53  | 1     | 646 | U    |
| 53  | 1     | 654 | A    |
| 53  | 1     | 669 | G    |
| 53  | 1     | 686 | U    |
| 53  | 1     | 687 | C    |
| 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    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 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     | 858  | G    |
| 53  | 1     | 860  | U    |
| 53  | 1     | 878  | A    |
| 53  | 1     | 887  | U    |
| 53  | 1     | 896  | A    |
| 53  | 1     | 897  | C    |
| 53  | 1     | 907  | G    |
| 53  | 1     | 910  | A    |
| 53  | 1     | 932  | U    |
| 53  | 1     | 941  | A    |
| 53  | 1     | 945  | A    |
| 53  | 1     | 946  | C    |
| 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     | 1046 | A    |
| 53  | 1     | 1047 | G    |
| 53  | 1     | 1054 | A    |
| 53  | 1     | 1060 | U    |
| 53  | 1     | 1062 | G    |
| 53  | 1     | 1066 | U    |
| 53  | 1     | 1070 | A    |
| 53  | 1     | 1071 | G    |
| 53  | 1     | 1079 | C    |
| 53  | 1     | 1084 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 1088 | A    |
| 53  | 1     | 1090 | A    |
| 53  | 1     | 1104 | C    |
| 53  | 1     | 1106 | G    |
| 53  | 1     | 1111 | A    |
| 53  | 1     | 1131 | G    |
| 53  | 1     | 1132 | U    |
| 53  | 1     | 1133 | A    |
| 53  | 1     | 1135 | C    |
| 53  | 1     | 1143 | A    |
| 53  | 1     | 1174 | U    |
| 53  | 1     | 1175 | A    |
| 53  | 1     | 1177 | G    |
| 53  | 1     | 1180 | U    |
| 53  | 1     | 1206 | G    |
| 53  | 1     | 1211 | C    |
| 53  | 1     | 1212 | G    |
| 53  | 1     | 1238 | 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     | 1289 | C    |
| 53  | 1     | 1301 | A    |
| 53  | 1     | 1329 | U    |
| 53  | 1     | 1330 | C    |
| 53  | 1     | 1332 | G    |
| 53  | 1     | 1345 | C    |
| 53  | 1     | 1352 | U    |
| 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    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 1476 | U    |
| 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    |
| 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     | 1800 | C    |
| 53  | 1     | 1801 | A    |
| 53  | 1     | 1802 | 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    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 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     | 1971 | U    |
| 53  | 1     | 1972 | G    |
| 53  | 1     | 1993 | U    |
| 53  | 1     | 1997 | C    |
| 53  | 1     | 2022 | U    |
| 53  | 1     | 2023 | C    |
| 53  | 1     | 2030 | A    |
| 53  | 1     | 2031 | A    |
| 53  | 1     | 2036 | C    |
| 53  | 1     | 2043 | C    |
| 53  | 1     | 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     | 2113 | U    |
| 53  | 1     | 2118 | U    |
| 53  | 1     | 2119 | A    |
| 53  | 1     | 2132 | U    |
| 53  | 1     | 2133 | G    |
| 53  | 1     | 2147 | A    |
| 53  | 1     | 2162 | G    |
| 53  | 1     | 2171 | A    |
| 53  | 1     | 2172 | U    |
| 53  | 1     | 2173 | A    |
| 53  | 1     | 2189 | U    |
| 53  | 1     | 2198 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 2203 | U    |
| 53  | 1     | 2204 | G    |
| 53  | 1     | 2213 | U    |
| 53  | 1     | 2225 | A    |
| 53  | 1     | 2238 | G    |
| 53  | 1     | 2239 | G    |
| 53  | 1     | 2268 | A    |
| 53  | 1     | 2278 | A    |
| 53  | 1     | 2283 | C    |
| 53  | 1     | 2287 | A    |
| 53  | 1     | 2297 | A    |
| 53  | 1     | 2305 | U    |
| 53  | 1     | 2309 | A    |
| 53  | 1     | 2325 | G    |
| 53  | 1     | 2327 | A    |
| 53  | 1     | 2334 | U    |
| 53  | 1     | 2350 | C    |
| 53  | 1     | 2383 | G    |
| 53  | 1     | 2385 | C    |
| 53  | 1     | 2392 | A    |
| 53  | 1     | 2402 | U    |
| 53  | 1     | 2406 | A    |
| 53  | 1     | 2423 | U    |
| 53  | 1     | 2424 | 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     | 2520 | C    |
| 53  | 1     | 2529 | G    |
| 53  | 1     | 2547 | A    |
| 53  | 1     | 2554 | U    |
| 53  | 1     | 2566 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 2567 | G    |
| 53  | 1     | 2572 | A    |
| 53  | 1     | 2602 | A    |
| 53  | 1     | 2603 | G    |
| 53  | 1     | 2609 | U    |
| 53  | 1     | 2613 | U    |
| 53  | 1     | 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    |
| 53  | 1     | 2779 | U    |
| 53  | 1     | 2791 | G    |
| 53  | 1     | 2794 | C    |
| 53  | 1     | 2797 | U    |
| 53  | 1     | 2800 | A    |
| 53  | 1     | 2809 | A    |
| 53  | 1     | 2820 | A    |
| 53  | 1     | 2821 | A    |
| 53  | 1     | 2833 | U    |
| 53  | 1     | 2867 | G    |
| 53  | 1     | 2872 | A    |
| 53  | 1     | 2879 | A    |
| 53  | 1     | 2880 | C    |
| 53  | 1     | 2883 | A    |
| 54  | 2     | 4    | C    |
| 54  | 2     | 12   | C    |
| 54  | 2     | 13   | G    |
| 54  | 2     | 24   | G    |
| 54  | 2     | 35   | C    |
| 54  | 2     | 41   | G    |
| 54  | 2     | 44   | G    |
| 54  | 2     | 67   | G    |
| 54  | 2     | 89   | U    |
| 54  | 2     | 90   | C    |
| 54  | 2     | 108  | A    |
| 54  | 2     | 109  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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  | 6     | 6   | G    |
| 55  | 6     | 9   | G    |
| 55  | 6     | 18  | G    |
| 55  | 6     | 19  | G    |
| 55  | 6     | 20  | U    |
| 55  | 6     | 47  | U    |
| 55  | 6     | 49  | G    |
| 55  | 6     | 61  | C    |
| 56  | 4     | 12  | A    |
| 56  | 4     | 13  | A    |
| 56  | 4     | 19  | U    |
| 57  | 7     | 8   | U    |
| 57  | 7     | 9   | A    |
| 57  | 7     | 10  | G    |
| 57  | 7     | 18  | G    |
| 57  | 7     | 21  | A    |
| 57  | 7     | 26  | A    |
| 57  | 7     | 45  | U    |
| 57  | 7     | 46  | G    |
| 57  | 7     | 48  | C    |
| 57  | 7     | 55  | U    |
| 57  | 7     | 59  | U    |
| 57  | 7     | 61  | C    |
| 57  | 7     | 63  | G    |
| 57  | 7     | 73  | A    |

All (16) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 52  | 3     | 421  | U    |
| 52  | 3     | 438  | U    |
| 52  | 3     | 495  | A    |
| 52  | 3     | 960  | U    |
| 52  | 3     | 1201 | A    |
| 53  | 1     | 421  | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | 1     | 490  | C    |
| 53  | 1     | 859  | G    |
| 53  | 1     | 1020 | A    |
| 53  | 1     | 1130 | U    |
| 53  | 1     | 1475 | G    |
| 53  | 1     | 2286 | G    |
| 53  | 1     | 2296 | U    |
| 53  | 1     | 2326 | C    |
| 53  | 1     | 2391 | G    |
| 54  | 2     | 88   | C    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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 | $\# Z  > 2$ |
| 61  | GTP  | 8     | 501 | -    | 33,34,34     | 0.93 | 1 (3%)      | 50,54,54    | 1.65 | 9 (18%)     |
| 59  | FME  | 5     | 101 | 55   | 8,9,10       | 0.47 | 0           | 8,9,11      | 1.03 | 1 (12%)     |
| 60  | PHE  | 7     | 101 | 57   | 10,11,12     | 0.72 | 0           | 8,13,15     | 0.26 | 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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 61  | GTP  | 8     | 501 | -    | -       | 5/22/38/38 | 0/3/3/3 |
| 59  | FME  | 5     | 101 | 55   | -       | 1/7/9/11   | -       |
| 60  | PHE  | 7     | 101 | 57   | -       | 0/5/6/8    | 0/1/1/1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 61  | 8     | 501 | GTP  | C2-N3 | 2.26 | 1.38        | 1.33     |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 61  | 8     | 501 | GTP  | C5-C4-N3    | -5.08 | 120.30      | 128.39   |
| 61  | 8     | 501 | GTP  | C2-N3-C4    | 4.74  | 120.46      | 112.30   |
| 61  | 8     | 501 | GTP  | N9-C4-N3    | 3.23  | 132.41      | 125.95   |
| 61  | 8     | 501 | GTP  | C2-N1-C6    | -3.02 | 119.63      | 125.11   |
| 61  | 8     | 501 | GTP  | C5-C6-N1    | 2.67  | 120.05      | 113.25   |
| 61  | 8     | 501 | GTP  | O6-C6-C5    | -2.60 | 119.67      | 126.53   |
| 61  | 8     | 501 | GTP  | N9-C8-N7    | -2.33 | 109.07      | 113.40   |
| 61  | 8     | 501 | GTP  | C8-N7-C5    | 2.29  | 108.34      | 104.26   |
| 61  | 8     | 501 | GTP  | C3'-C2'-C1' | 2.27  | 105.76      | 101.46   |
| 59  | 5     | 101 | FME  | O-C-CA      | -2.01 | 119.61      | 124.77   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

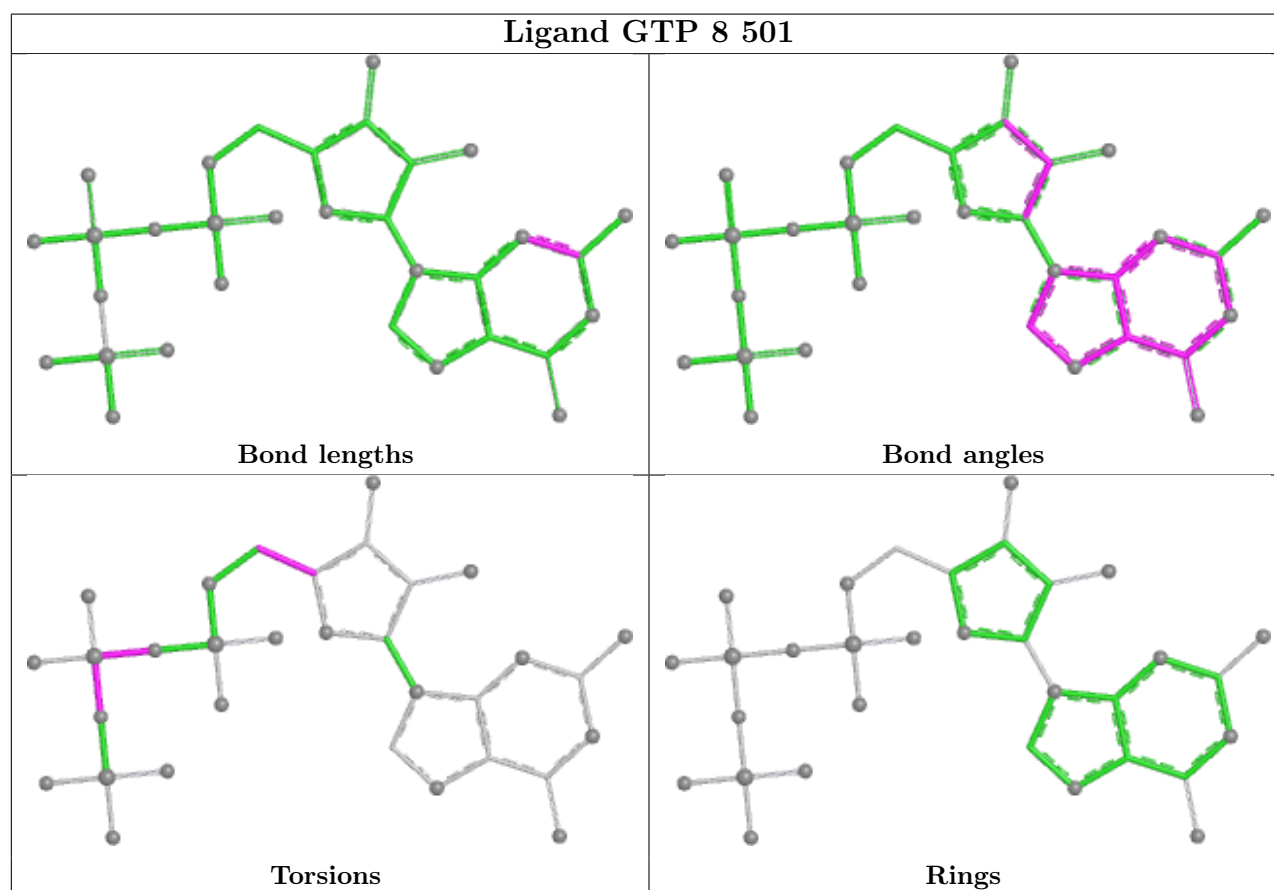
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 59  | 5     | 101 | FME  | O1-CN-N-CA      |
| 61  | 8     | 501 | GTP  | PG-O3B-PB-O2B   |
| 61  | 8     | 501 | GTP  | PA-O3A-PB-O1B   |
| 61  | 8     | 501 | GTP  | O4'-C4'-C5'-O5' |
| 61  | 8     | 501 | GTP  | PG-O3B-PB-O1B   |
| 61  | 8     | 501 | GTP  | PA-O3A-PB-O2B   |

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 61  | 8     | 501 | GTP  | 1       | 0            |
| 60  | 7     | 101 | PHE  | 1       | 0            |

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

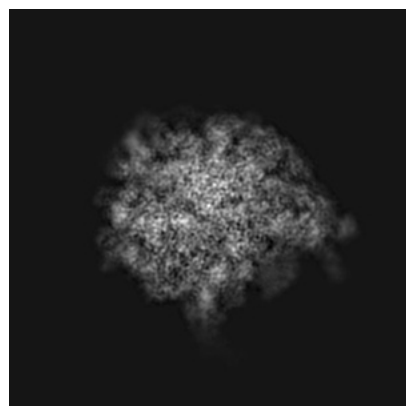
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21621. These allow visual inspection of the internal detail of the map and identification of artifacts.

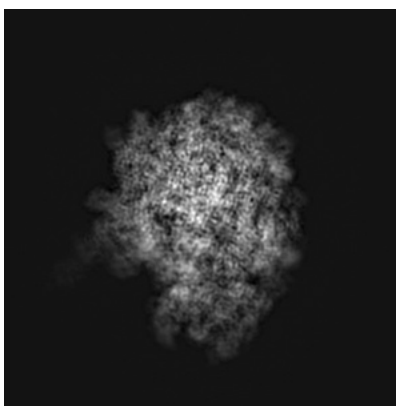
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

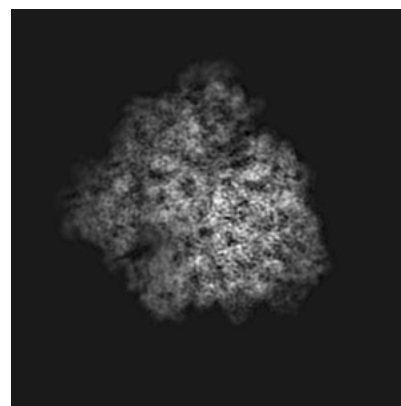
#### 6.1.1 Primary map



X

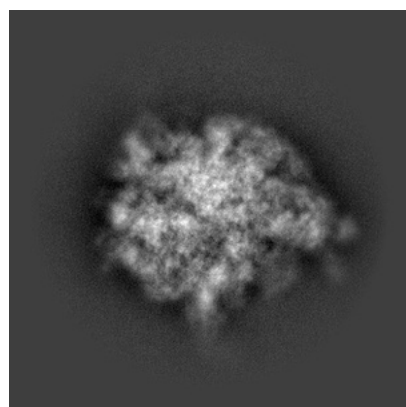


Y

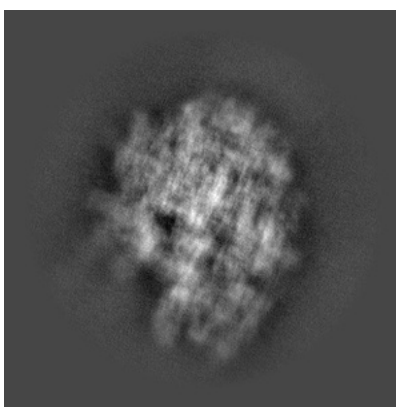


Z

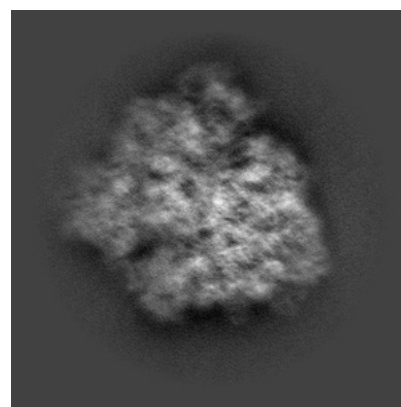
#### 6.1.2 Raw map



X



Y

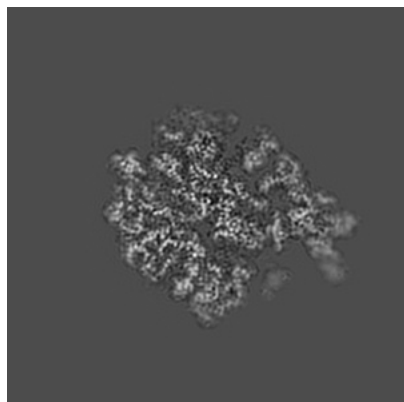


Z

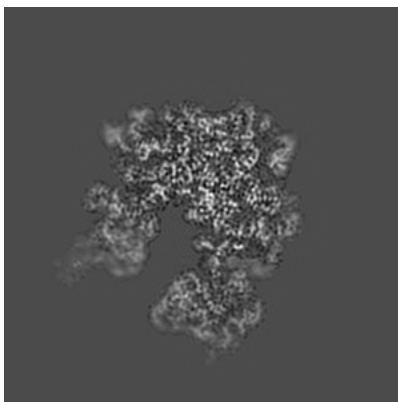
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

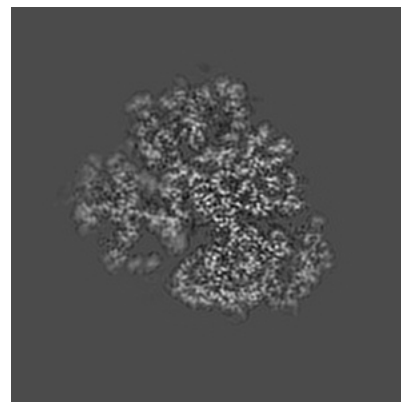
### 6.2.1 Primary map



X Index: 144

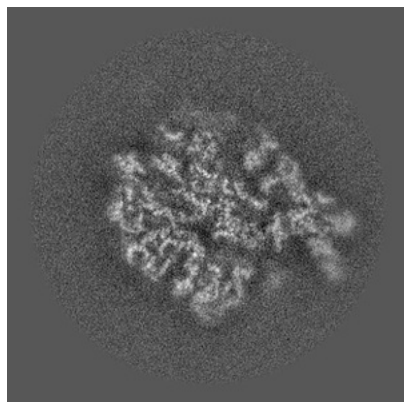


Y Index: 144

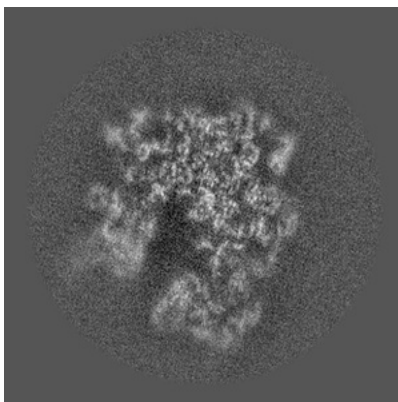


Z Index: 144

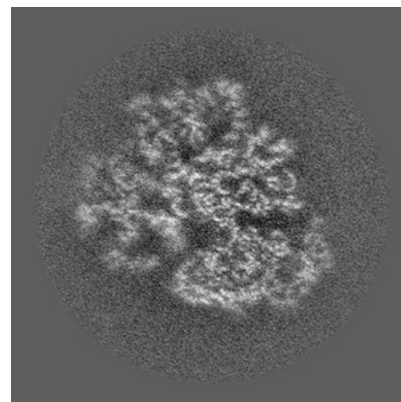
### 6.2.2 Raw map



X Index: 144



Y Index: 144



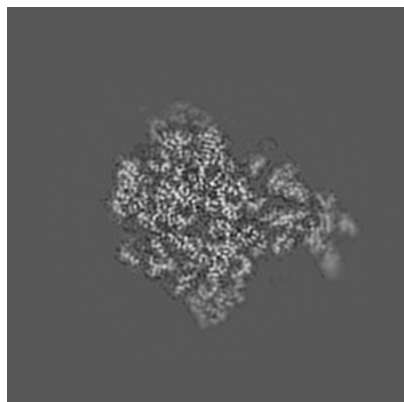
Z Index: 144

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

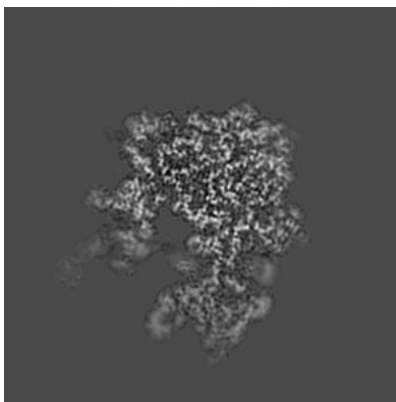


## 6.3 Largest variance slices [i](#)

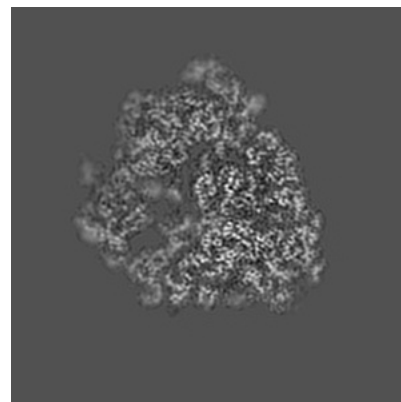
### 6.3.1 Primary map



X Index: 149

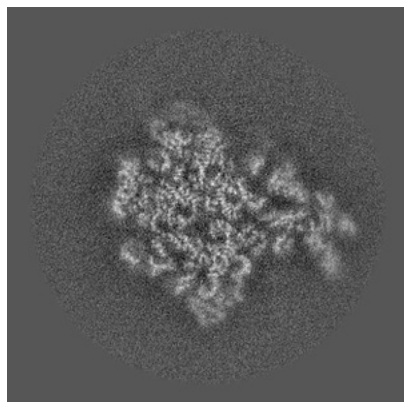


Y Index: 151

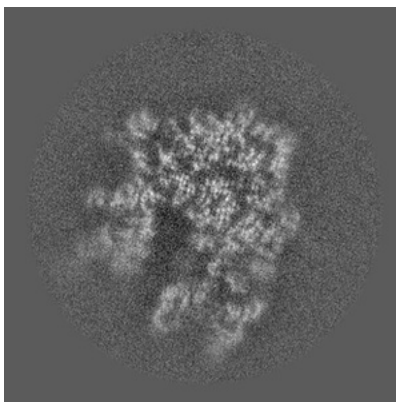


Z Index: 135

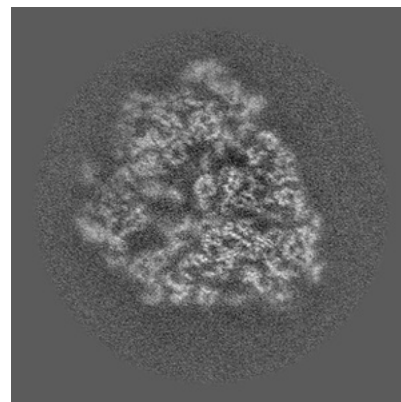
### 6.3.2 Raw map



X Index: 149



Y Index: 148

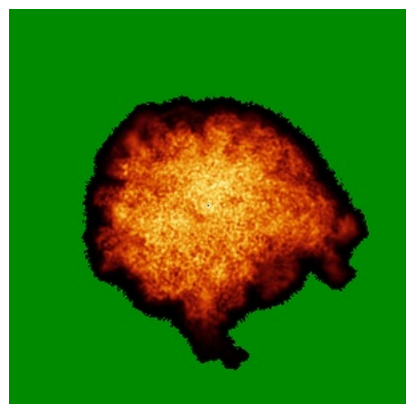


Z Index: 135

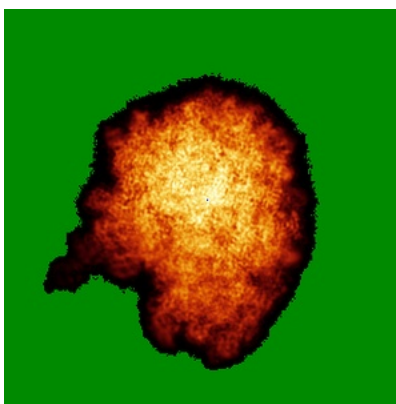
The images above show the largest variance slices of the map in three orthogonal directions.

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

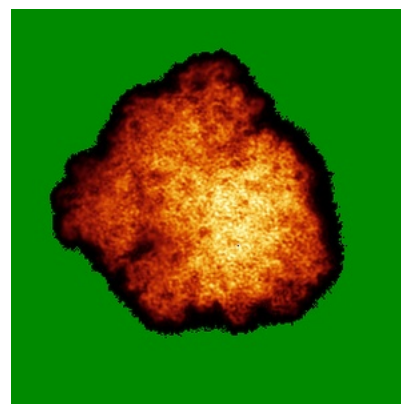
### 6.4.1 Primary map



X

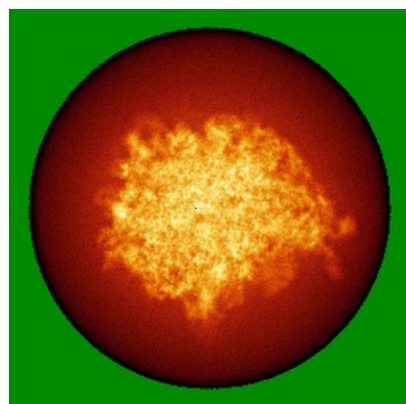


Y

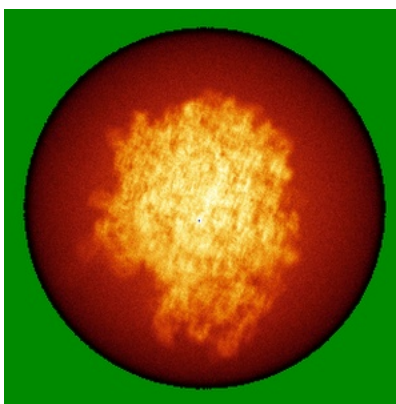


Z

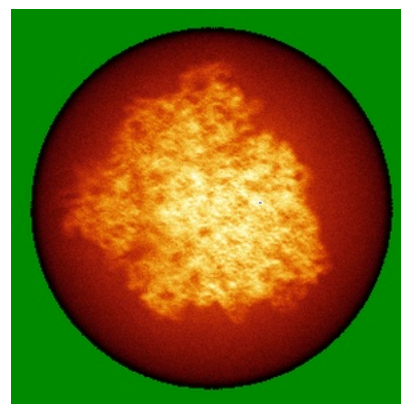
### 6.4.2 Raw map



X



Y



Z

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

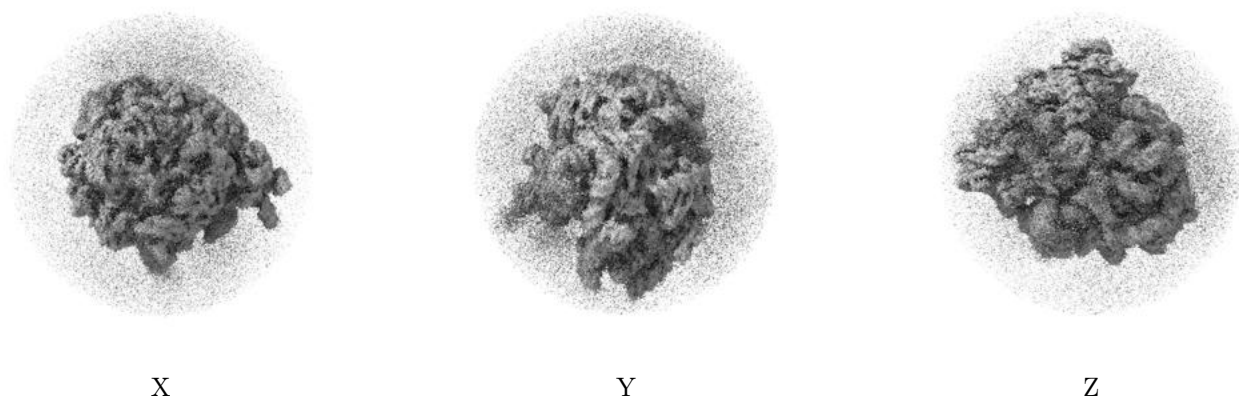
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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

### 6.5.2 Raw map



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

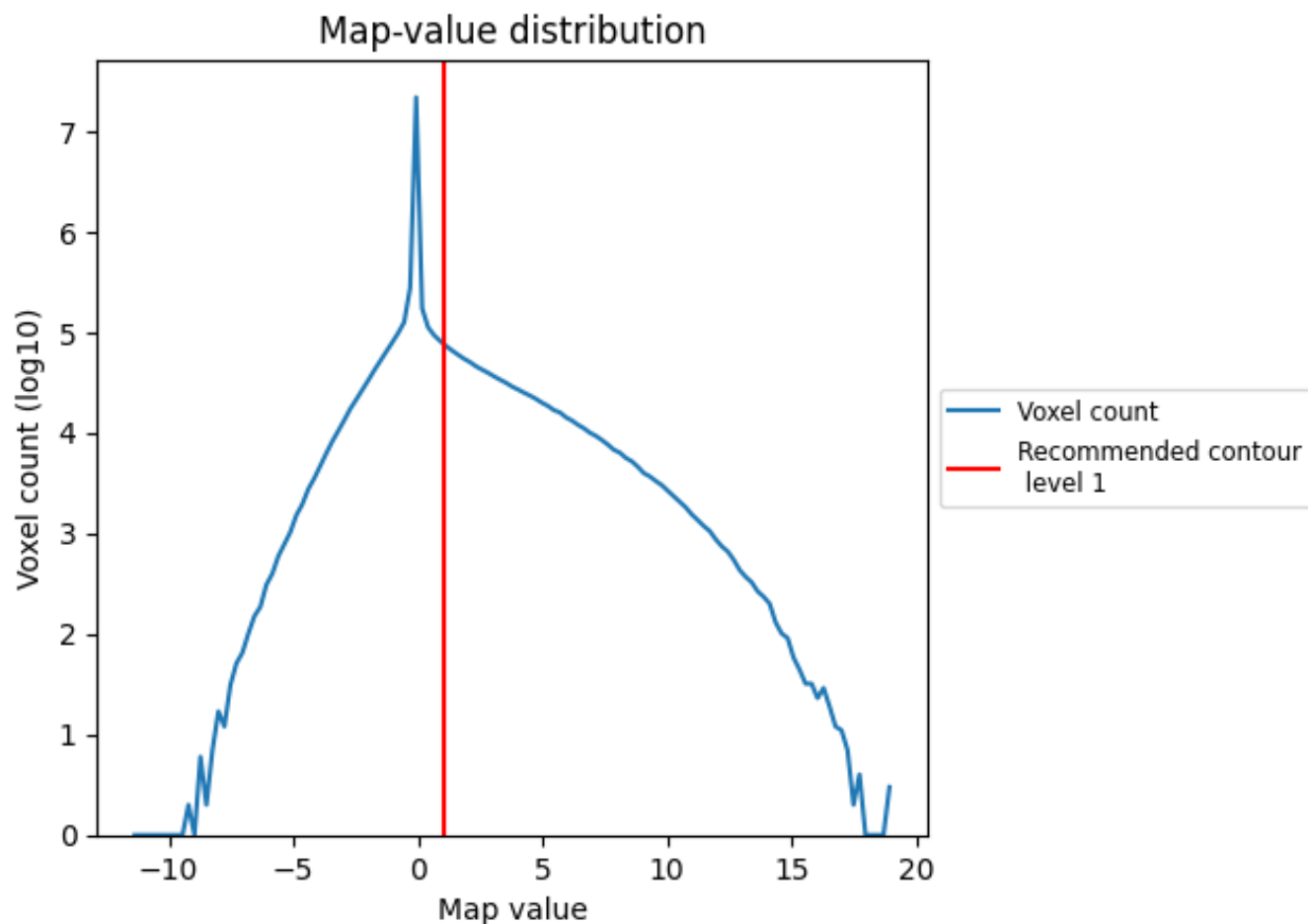
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

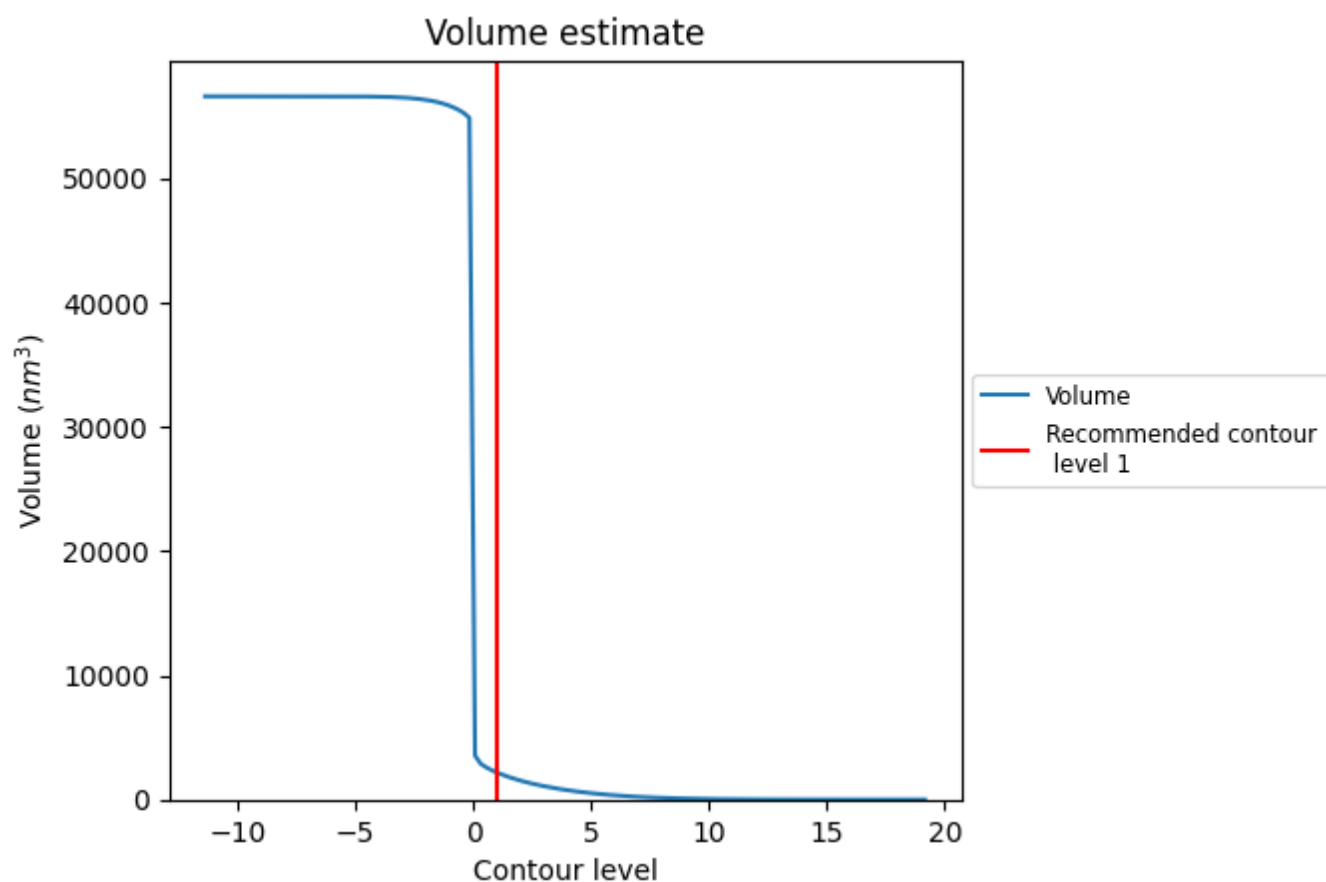
This section contains the results of statistical analysis of the map.

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



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

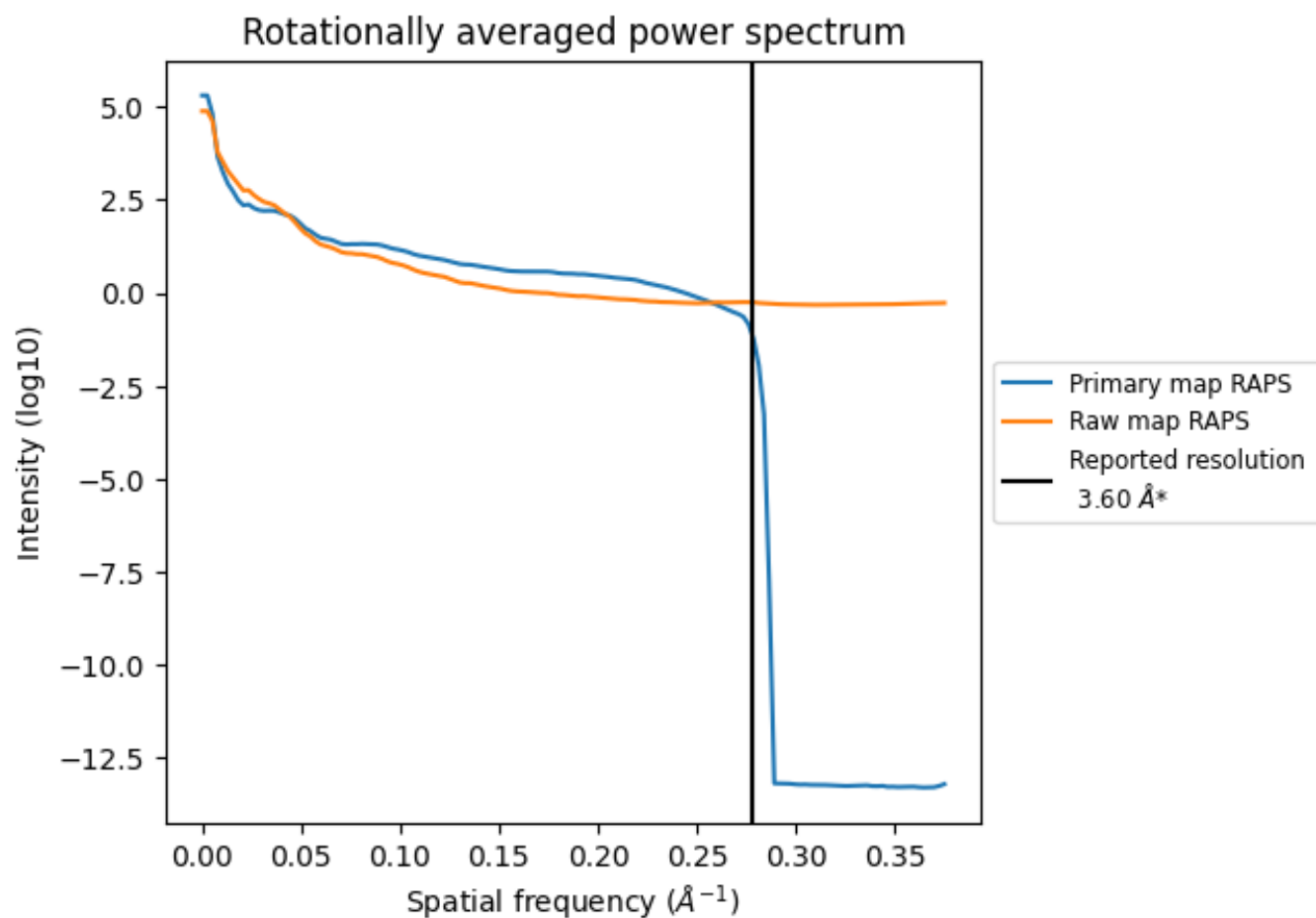
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2178 nm<sup>3</sup>; this corresponds to an approximate mass of 1968 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

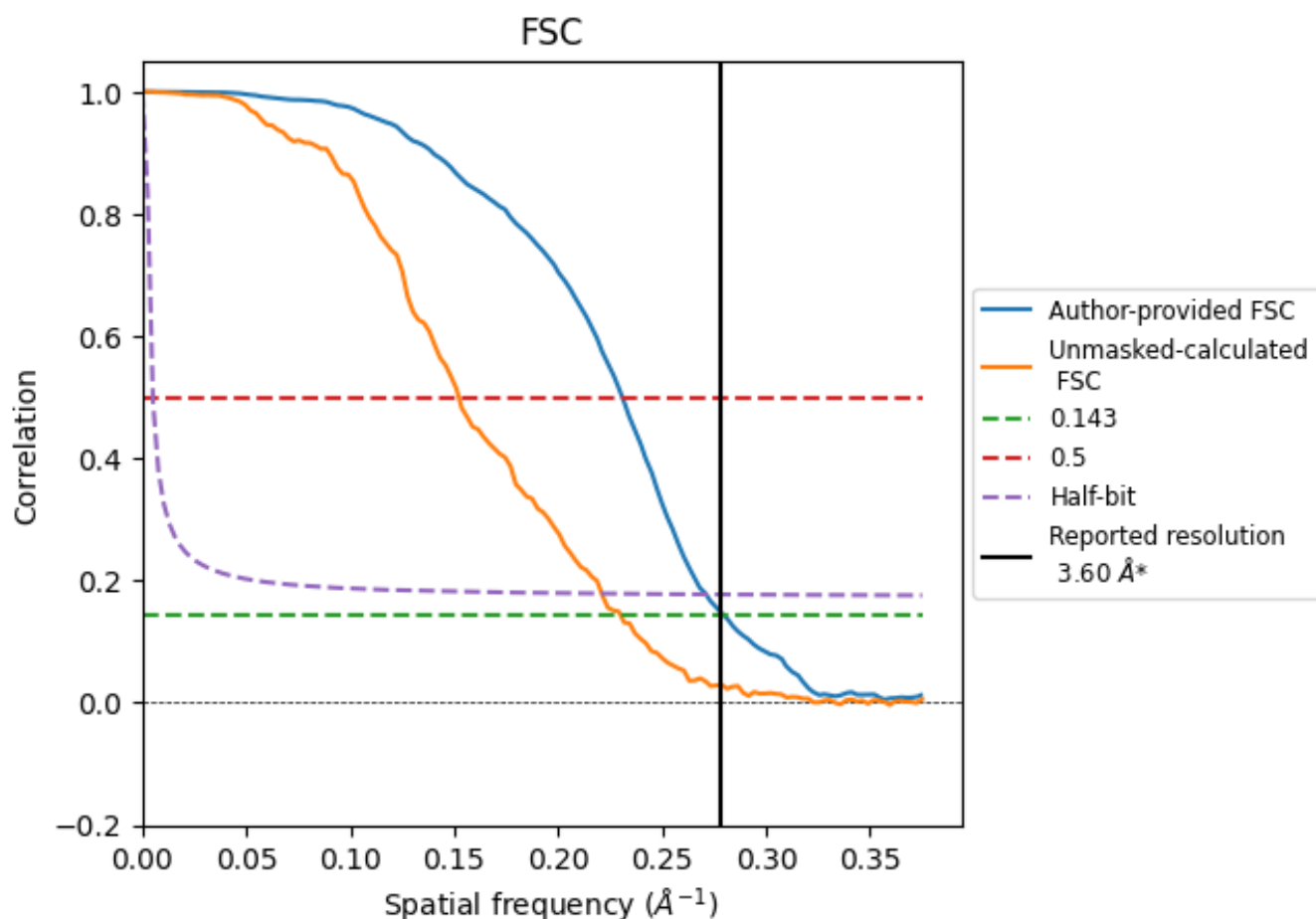


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.278  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.60                               | -    | -        |
| Author-provided FSC curve | 3.58                               | 4.33 | 3.69     |
| Unmasked-calculated*      | 4.35                               | 6.57 | 4.52     |

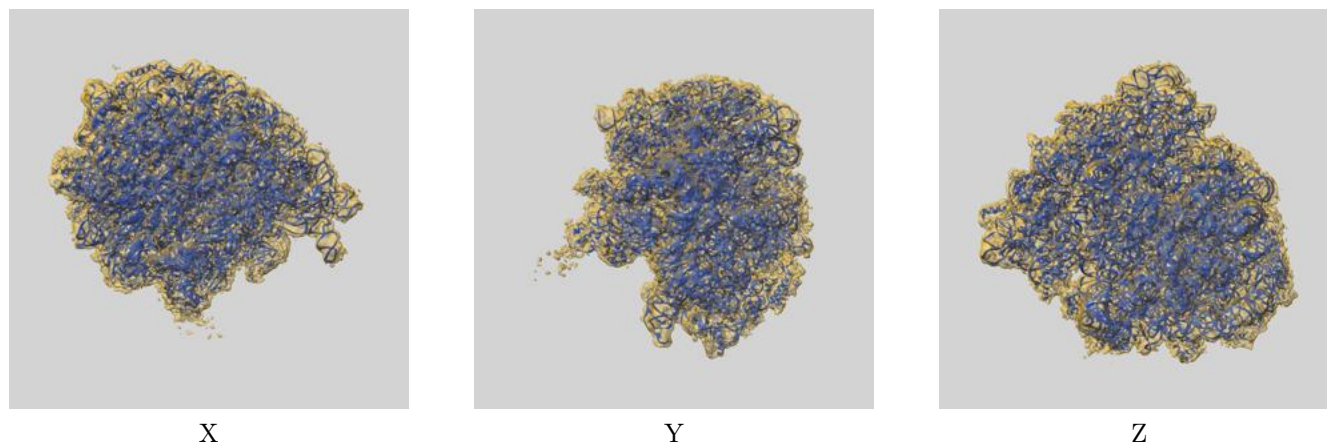
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 3.6 by more than 10 %



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

This section contains information regarding the fit between EMDB map EMD-21621 and PDB model 6WD2. Per-residue inclusion information can be found in section [3](#) on page [17](#).

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



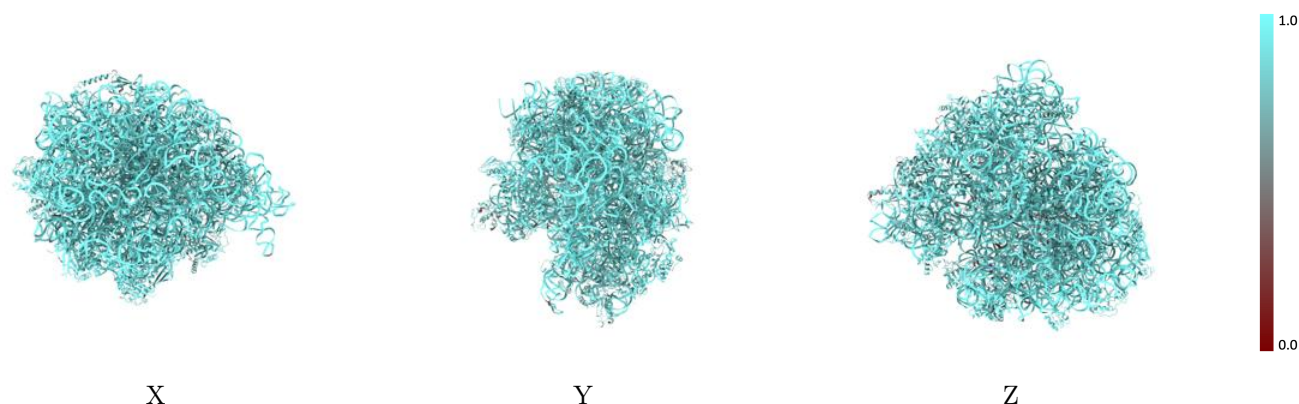
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



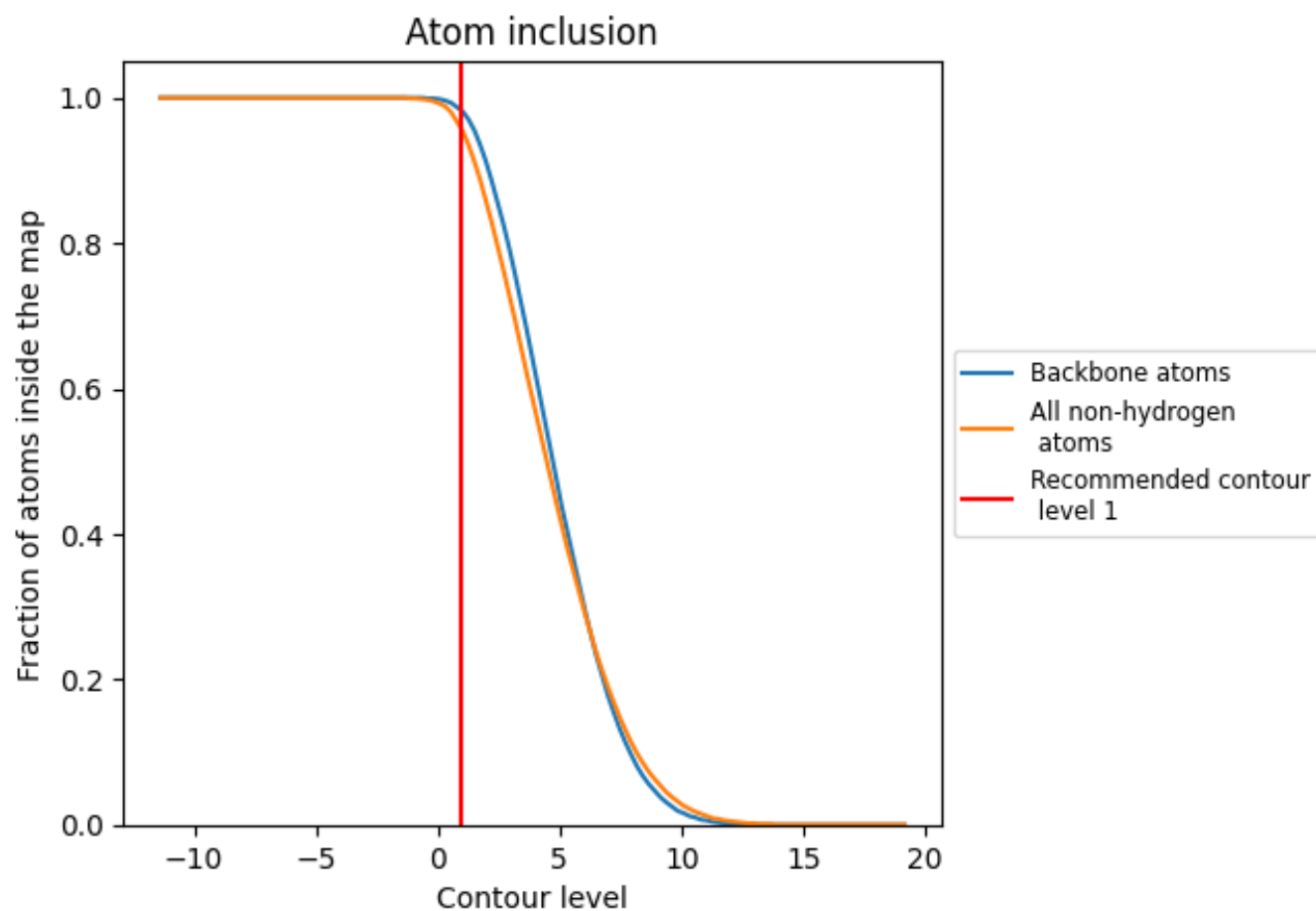
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

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

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9560   |  0.3660   |
| 1     |  0.9850   |  0.3880   |
| 2     |  0.9910   |  0.3470   |
| 3     |  0.9790   |  0.3570   |
| 4     |  0.8380   |  0.2190   |
| 5     |  0.9670   |  0.3150   |
| 6     |  0.8360   |  0.1380   |
| 7     |  0.9180   |  0.1780   |
| 8     |  0.8900   |  0.2010   |
| B     |  0.9320   |  0.4420   |
| C     |  0.8430   |  0.3680   |
| D     |  0.9470   |  0.4520   |
| E     |  0.9470   |  0.4710   |
| F     |  0.9040   |  0.4300   |
| G     |  0.8850  |  0.3140  |
| H     |  0.8130 |  0.3150 |
| I     |  0.8690 |  0.3230 |
| J     |  0.9150 |  0.3970 |
| K     |  0.9490 |  0.3740 |
| L     |  0.9160 |  0.3260 |
| M     |  0.9320 |  0.4080 |
| N     |  0.8880 |  0.3210 |
| O     |  0.7680 |  0.3110 |
| P     |  0.9460 |  0.3850 |
| Q     |  0.9110 |  0.4120 |
| R     |  0.9270 |  0.3350 |
| S     |  0.8270 |  0.3170 |
| T     |  0.9620 |  0.3930 |
| U     |  0.8980 |  0.3770 |
| V     |  0.9260 |  0.3980 |
| W     |  0.9220 |  0.3530 |
| X     |  0.9490 |  0.2980 |
| Y     |  0.9120 |  0.3570 |
| Z     |  0.8650 |  0.3270 |
| a     |  0.8450 |  0.1580 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| b     |  0.9490   |  0.4620   |
| c     |  0.9620   |  0.4540   |
| d     |  0.9470   |  0.4140   |
| e     |  0.9350   |  0.3310   |
| f     |  0.9520   |  0.3730   |
| g     |  0.7920   |  0.2830   |
| h     |  0.7410   |  0.1680   |
| i     |  0.7980   |  0.1810   |
| j     |  0.9430   |  0.4390   |
| k     |  0.9320   |  0.4450   |
| l     |  0.9440   |  0.4370   |
| m     |  0.9290   |  0.4330   |
| n     |  0.9370   |  0.4440   |
| o     |  0.9540   |  0.3650   |
| p     |  0.9360   |  0.4340   |
| q     |  0.9440   |  0.4400   |
| r     |  0.9600   |  0.4250   |
| s     |  0.9330  |  0.4480  |
| t     |  0.9380 |  0.4200 |
| u     |  0.9390 |  0.3840 |
| v     |  0.9540 |  0.4050 |
| w     |  0.9620 |  0.4530 |
| x     |  0.9580 |  0.4340 |
| y     |  0.9380 |  0.3480 |
| z     |  0.9540 |  0.4440 |