



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:18 AM UTC

PDB ID : 6BU8 / pdb\_00006bu8  
EMDB ID : EMD-7289  
Title : 70S ribosome with S1 domains 1 and 2 (Class 1)  
Authors : Loveland, A.B.; Korostelev, A.A.  
Deposited on : 2017-12-08  
Resolution : 3.50 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

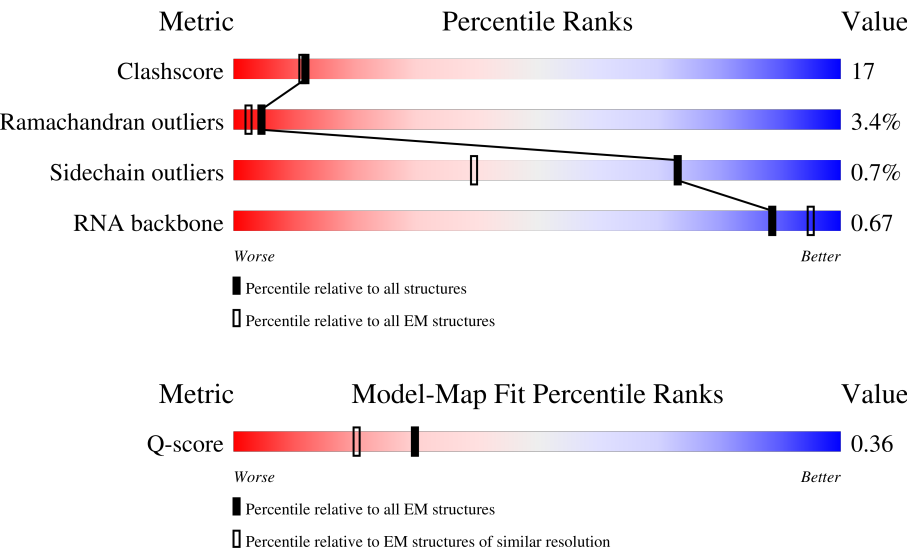
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 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.



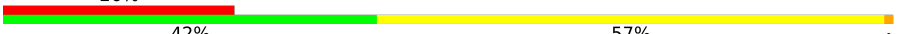
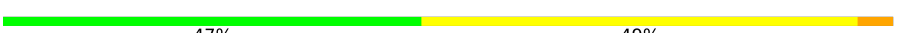
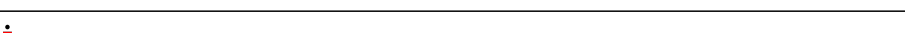
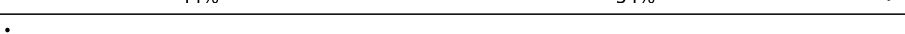
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 13950 ( 3.00 - 4.00 )                                    |

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   | 04    | 271    | <div> <div>48%</div> <div>49%</div> <div>.</div> </div> |
| 2   | 05    | 209    | <div> <div>56%</div> <div>43%</div> </div>              |
| 3   | 06    | 201    | <div> <div>48%</div> <div>50%</div> <div>.</div> </div> |

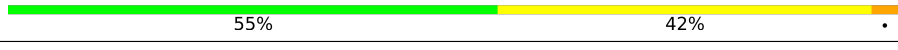
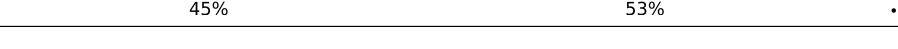
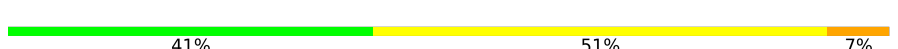
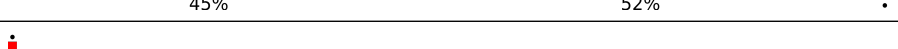
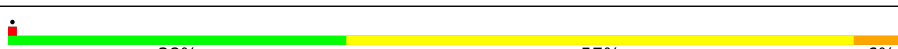
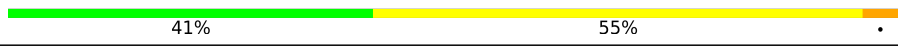
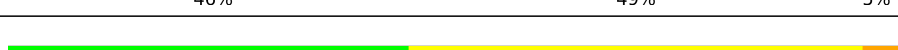
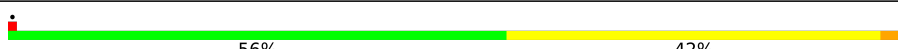
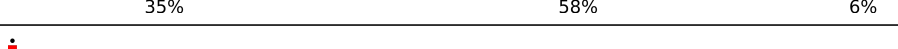
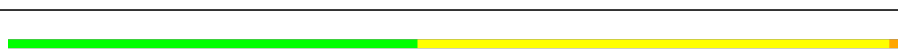
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | 07    | 177    |    |
| 5   | 08    | 176    |    |
| 6   | 09    | 149    |    |
| 7   | 10    | 131    |    |
| 8   | 11    | 141    |    |
| 9   | 12    | 142    |    |
| 10  | 13    | 122    |    |
| 11  | 14    | 143    |    |
| 12  | 15    | 136    |    |
| 13  | 16    | 120    |    |
| 14  | 17    | 116    |    |
| 15  | 18    | 114    |    |
| 16  | 19    | 117    |  |
| 17  | 20    | 103    |  |
| 18  | 21    | 110    |  |
| 19  | 22    | 93     |  |
| 20  | 23    | 102    |  |
| 21  | 24    | 94     |  |
| 22  | 25    | 75     |  |
| 23  | 26    | 77     |  |
| 24  | 27    | 63     |  |
| 25  | 28    | 58     |  |
| 26  | 29    | 66     |  |
| 27  | 30    | 56     |  |
| 28  | 31    | 50     |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | 32    | 46     |    |
| 30  | 33    | 64     |    |
| 31  | 34    | 38     |    |
| 32  | B     | 225    |    |
| 33  | C     | 206    |    |
| 34  | D     | 205    |    |
| 35  | E     | 157    |    |
| 36  | F     | 126    |    |
| 37  | G     | 151    |    |
| 38  | H     | 129    |   |
| 39  | I     | 127    |  |
| 40  | J     | 98     |  |
| 41  | K     | 116    |  |
| 42  | L     | 123    |  |
| 43  | M     | 114    |  |
| 44  | N     | 100    |  |
| 45  | O     | 88     |  |
| 46  | P     | 82     |  |
| 47  | Q     | 80     |  |
| 48  | R     | 65     |  |
| 49  | S     | 79     |  |
| 50  | T     | 85     |  |
| 51  | U     | 65     |  |
| 52  | 03    | 223    |  |
| 53  | A     | 1539   |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 54  | 01    | 2903   |  |
| 55  | 02    | 120    |  |
| 56  | W     | 77     |  |
| 56  | X     | 77     |  |
| 57  | V     | 27     |  |
| 58  | Y     | 76     |  |
| 59  | Z     | 554    |  |

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 152151 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   | 04    | 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   | 05    | 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   | 06    | 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   | 07    | 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   | 08    | 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   | 09    | 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   | 10    | 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   | 11    | 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   | 12    | 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  | 13    | 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  | 14    | 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  | 15    | 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  | 16    | 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  | 17    | 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  | 18    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 16  | 19    | 117      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | 20    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | 21    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | 22    | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 739   | 466 | 139 | 132 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 20  | 23    | 102      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 780   | 492 | 146 | 142 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | 24    | 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  | 25    | 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  | 26    | 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  | 27    | 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  | 28    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | 29    | 66       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 523   | 323 | 99 | 95 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 27  | 30    | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 28  | 31    | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 410   | 263 | 75 | 72 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29  | 32    | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 30  | 33    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31  | 34    | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 32  | B     | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1757  | 1111 | 315 | 323 | 8 |         |       |

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | F     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1028  | 638 | 189 | 194 | 7 |         |       |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | 03    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1027  | 645 | 186 | 194 | 2 |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 54  | 01    | 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    |
|-------|---------|----------|--------|----------------|--------------|
| 01    | 747     | C        | U      | SEE REMARK 999 | GB 802133627 |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 55  | 02    | 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     |
|-------|---------|----------|--------|----------------|---------------|
| 02    | 120     | A        | -      | SEE REMARK 999 | GB 1266961702 |

- Molecule 56 is a RNA chain called tRNAfMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 56  | X     | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |       |
| 56  | W     | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |       |

- Molecule 57 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 57  | V     | 18       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 388   | 175 | 76 | 120 | 17 |         |       |

- Molecule 58 is a RNA chain called tRNAPhe.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 58  | Y     | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1622  | 723 | 290 | 533 | 76 |         |       |

- Molecule 59 is a protein called 30S ribosomal protein S1.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 59  | Z     | 156      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1204  | 760 | 209 | 235 |         |       |

- Molecule 60 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).

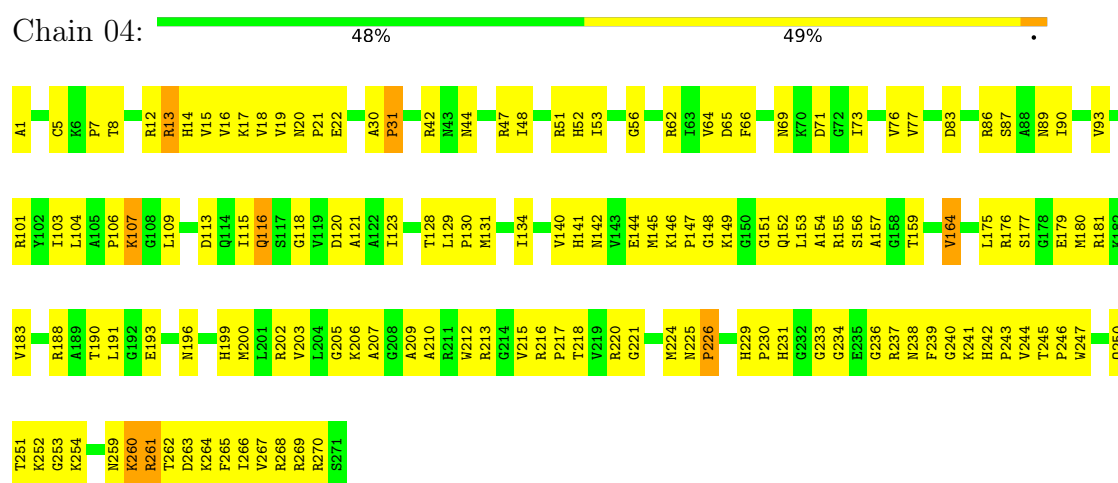


| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
|     |       |          | Total | C | N | O | S |         |
| 60  | W     | 1        | 10    | 6 | 1 | 2 | 1 | 0       |

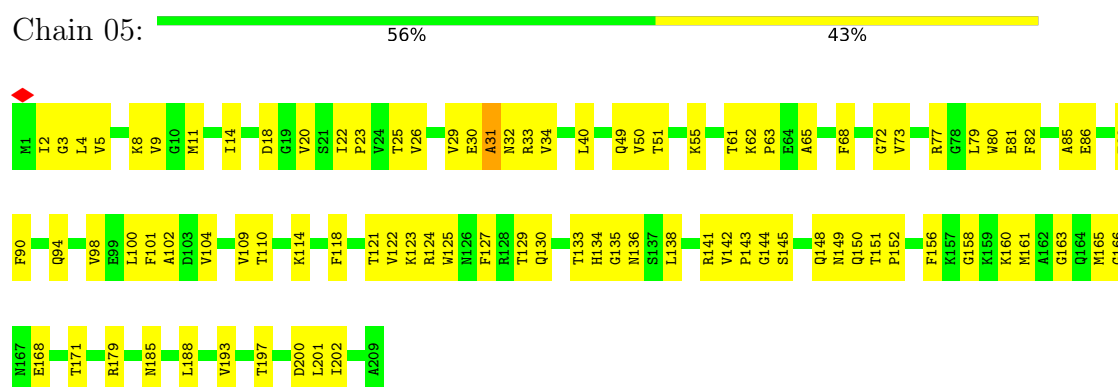
### 3 Residue-property plots

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

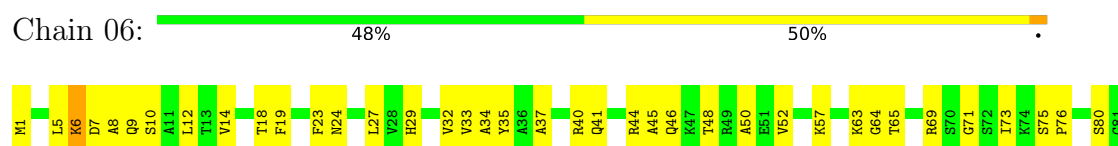
#### • Molecule 1: 50S ribosomal protein L2

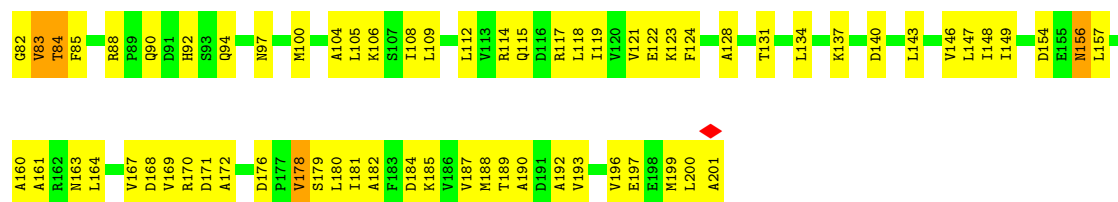


#### • Molecule 2: 50S ribosomal protein L3



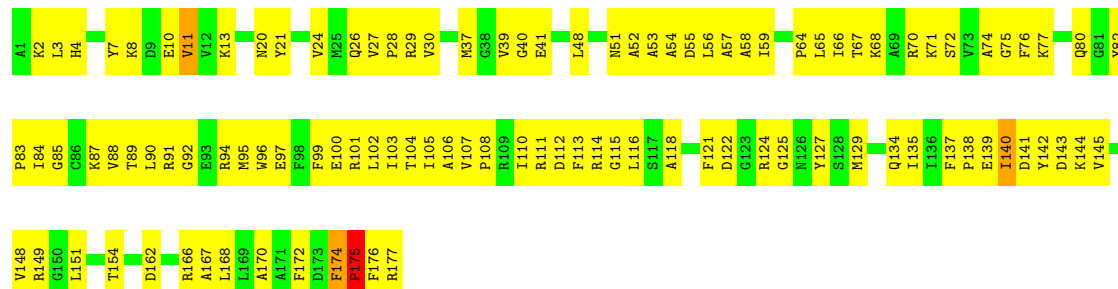
#### • Molecule 3: 50S ribosomal protein L4





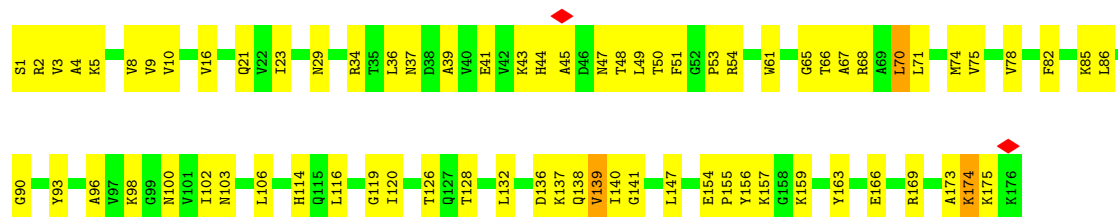
• Molecule 4: 50S ribosomal protein L5

Chain 07: 40% 58% ..



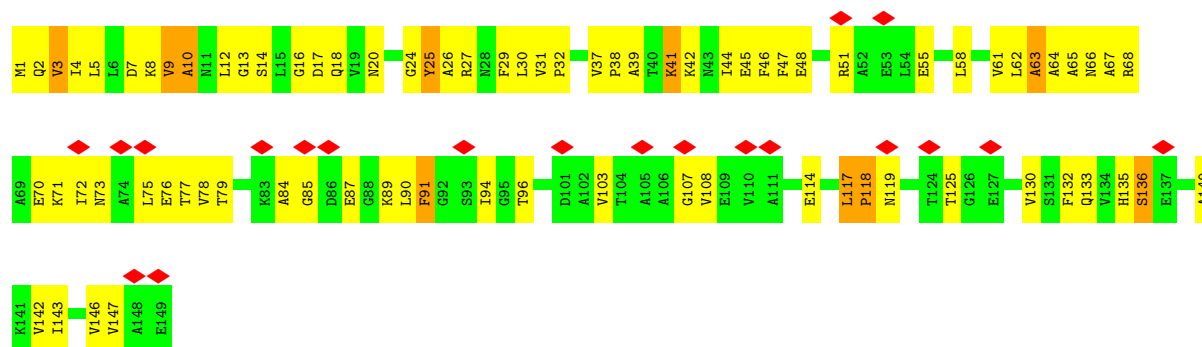
• Molecule 5: 50S ribosomal protein L6

Chain 08: 59% 40% .



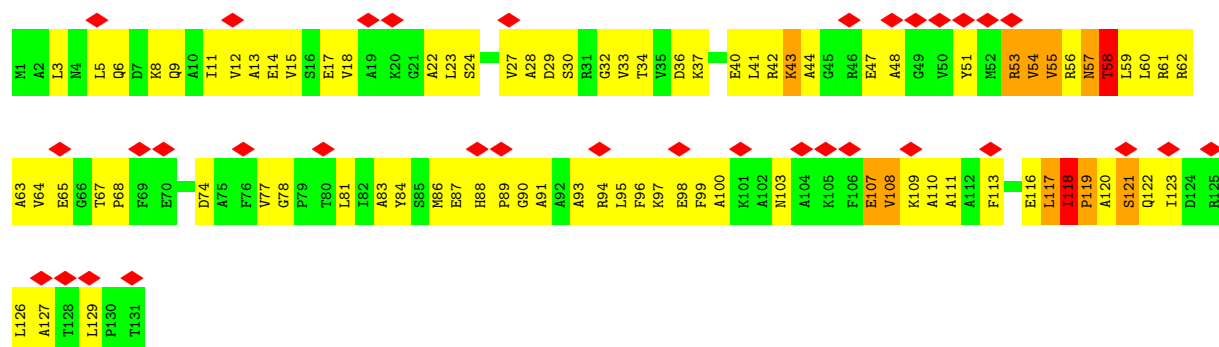
• Molecule 6: 50S ribosomal protein L9

Chain 09: 13% 46% 47% 7%

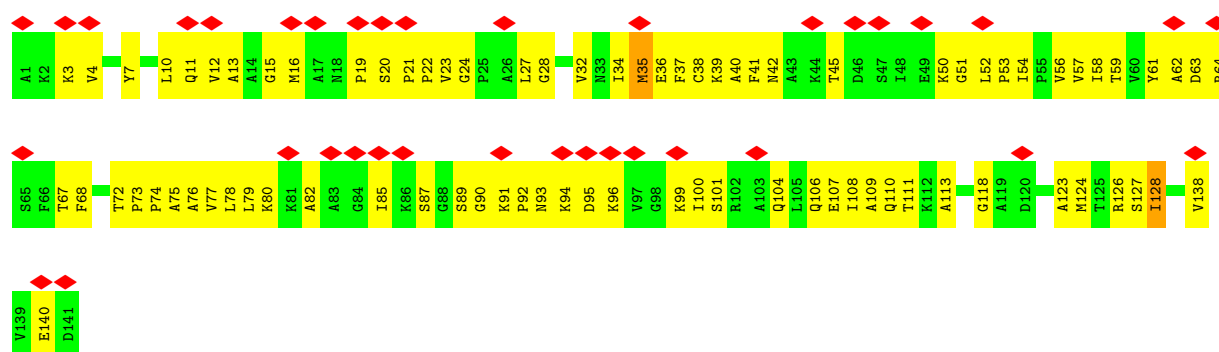
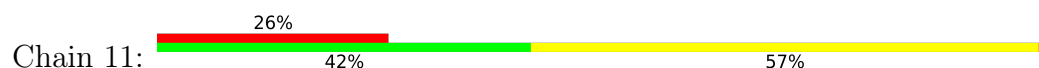


• Molecule 7: 50S ribosomal protein L10

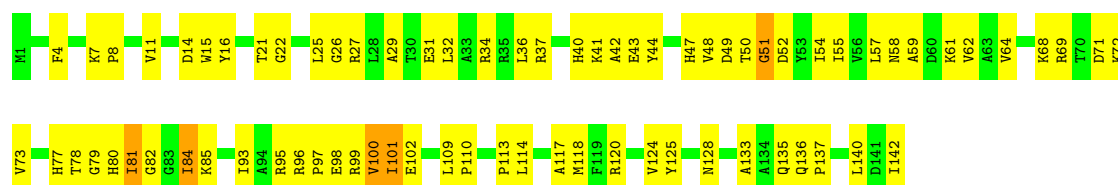
Chain 10: 26% 35% 56% 8%



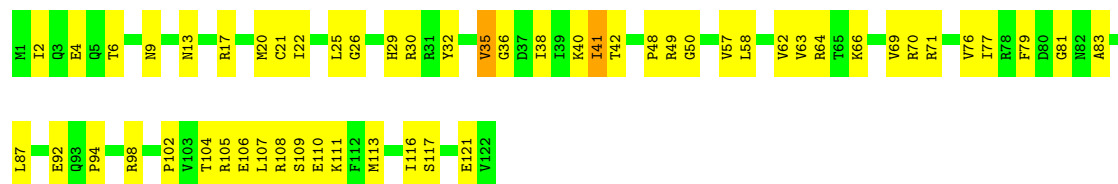
• Molecule 8: 50S ribosomal protein L11



• Molecule 9: 50S ribosomal protein L13

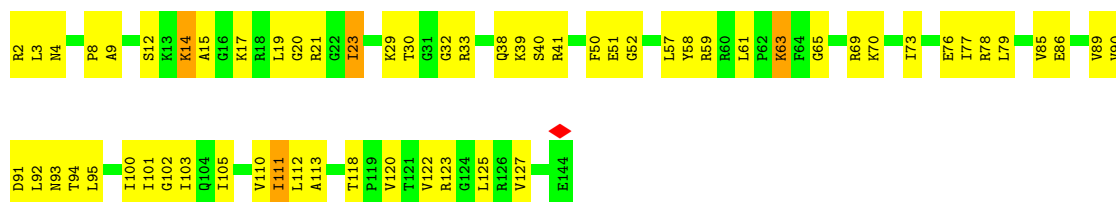


• Molecule 10: 50S ribosomal protein L14

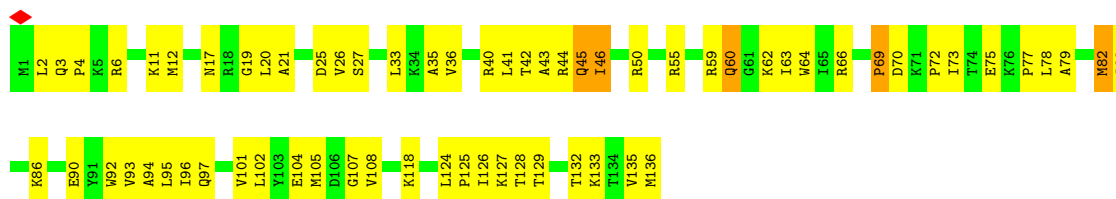


• Molecule 11: 50S ribosomal protein L15

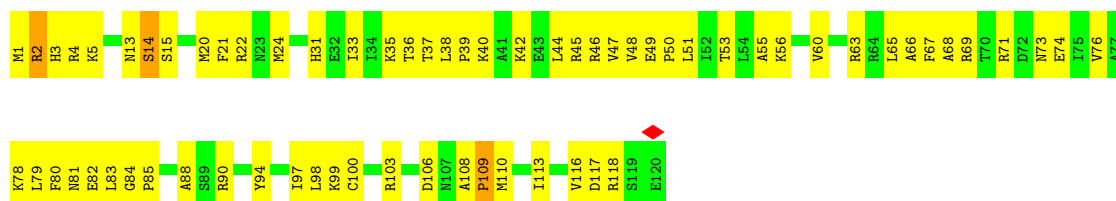




- Molecule 12: 50S ribosomal protein L16



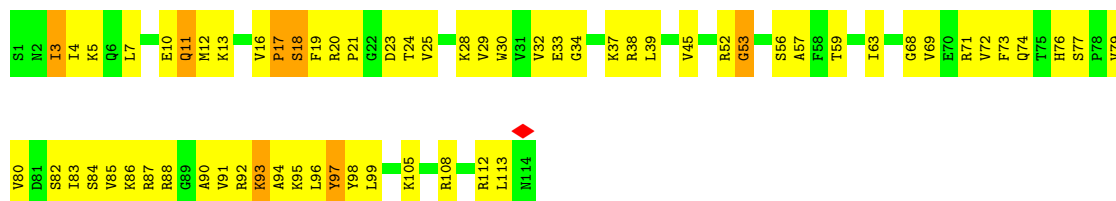
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18



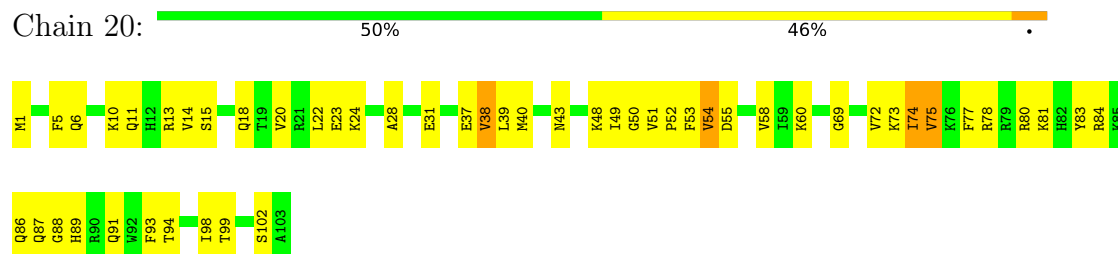
- Molecule 15: 50S ribosomal protein L19



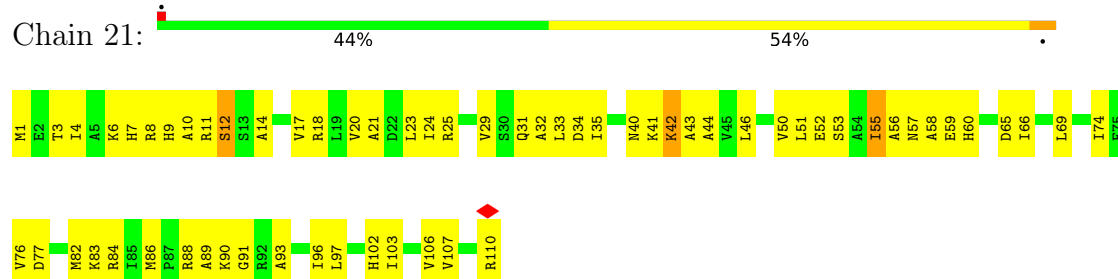
- Molecule 16: 50S ribosomal protein L20



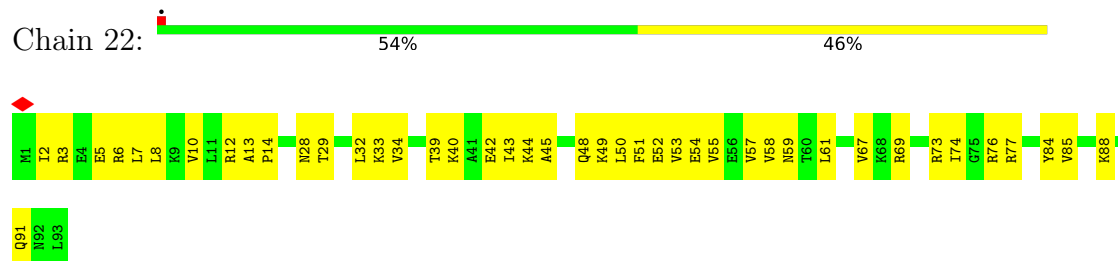
- Molecule 17: 50S ribosomal protein L21



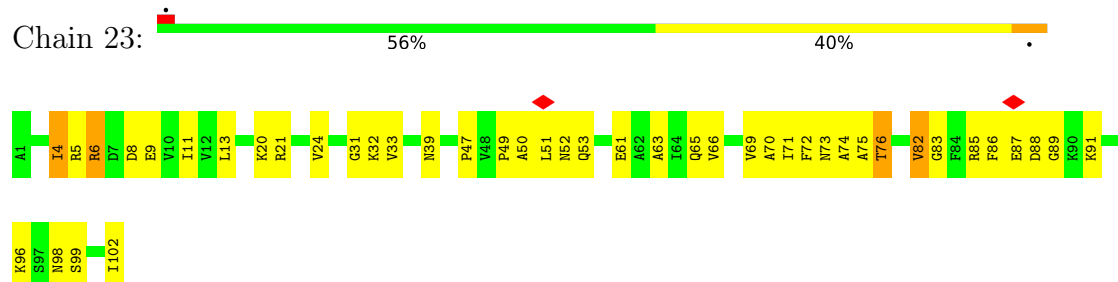
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



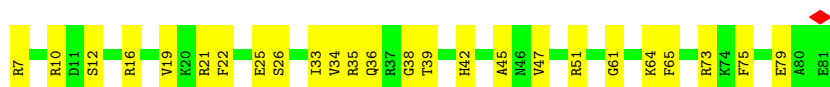
- Molecule 21: 50S ribosomal protein L25

Chain 24:  62% 37%



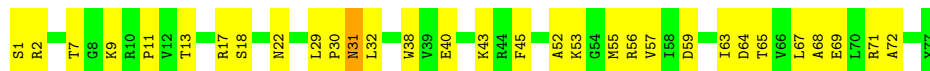
- Molecule 22: 50S ribosomal protein L27

Chain 25:  67% 33%



- Molecule 23: 50S ribosomal protein L28

Chain 26:  60% 39%



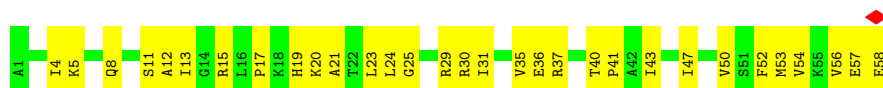
- Molecule 24: 50S ribosomal protein L29

Chain 27:  5% 51% 44% 5%



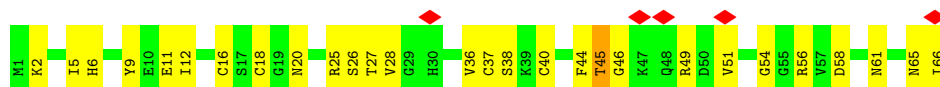
- Molecule 25: 50S ribosomal protein L30

Chain 28:  47% 53%

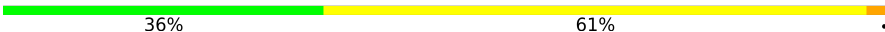


- Molecule 26: 50S ribosomal protein L31

Chain 29:  8% 58% 41%



- Molecule 27: 50S ribosomal protein L32

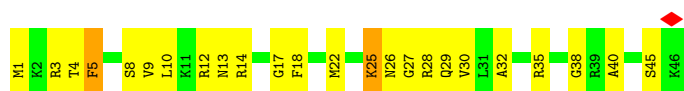
Chain 30:  36% 61%



- Molecule 28: 50S ribosomal protein L33



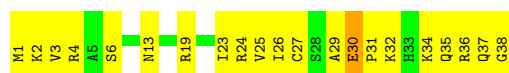
- Molecule 29: 50S ribosomal protein L34



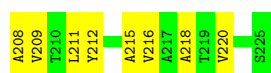
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36



- Molecule 32: 30S ribosomal protein S2

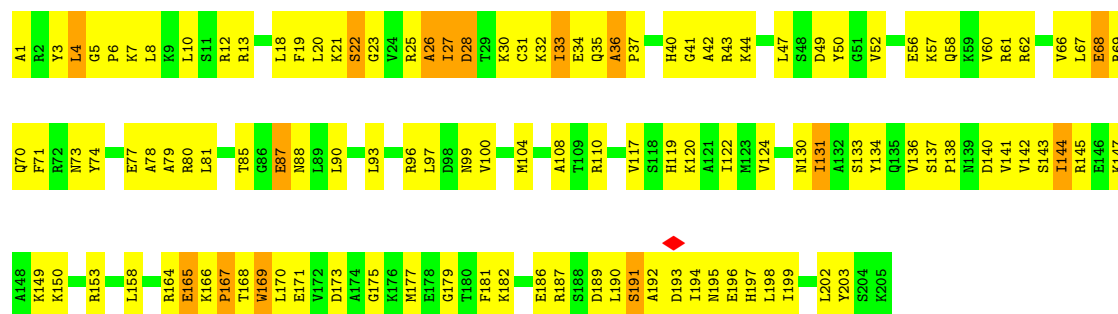


- Molecule 33: 30S ribosomal protein S3

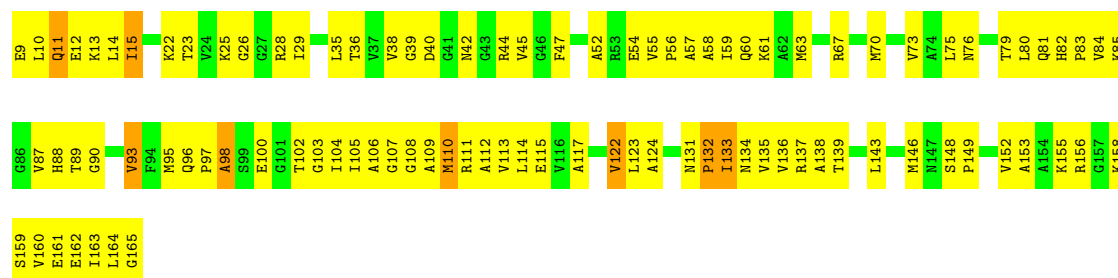




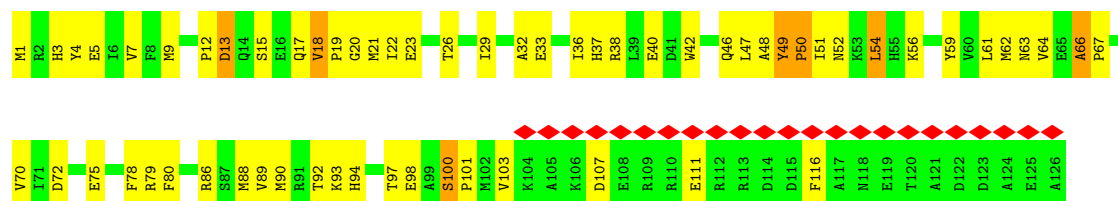
• Molecule 34: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S5

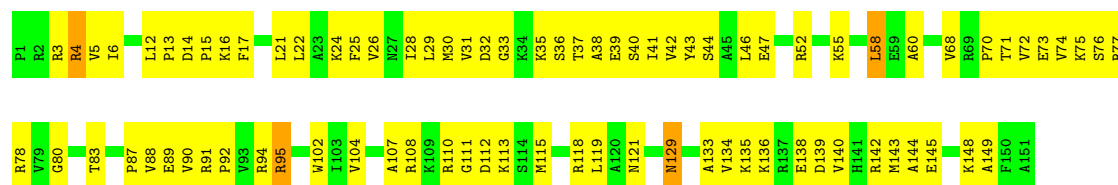


• Molecule 36: 30S ribosomal protein S6

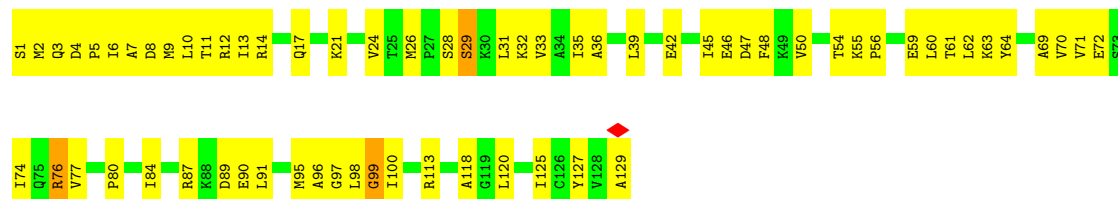


• Molecule 37: 30S ribosomal protein S7

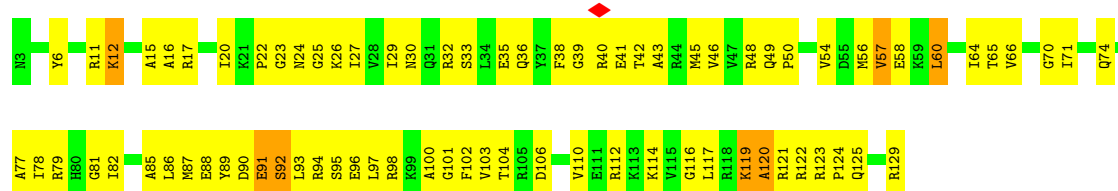




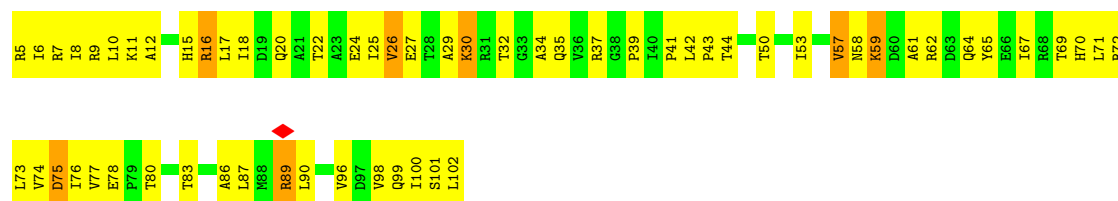
• Molecule 38: 30S ribosomal protein S8



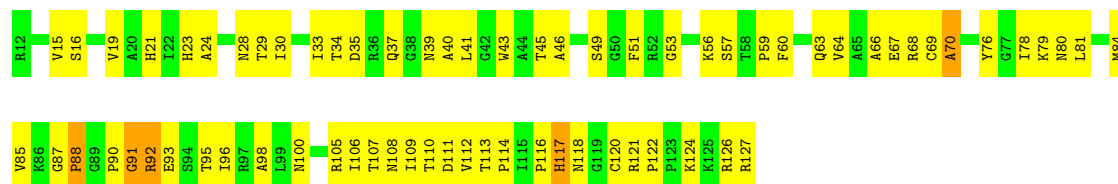
• Molecule 39: 30S ribosomal protein S9



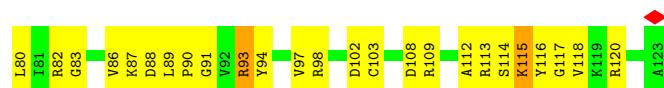
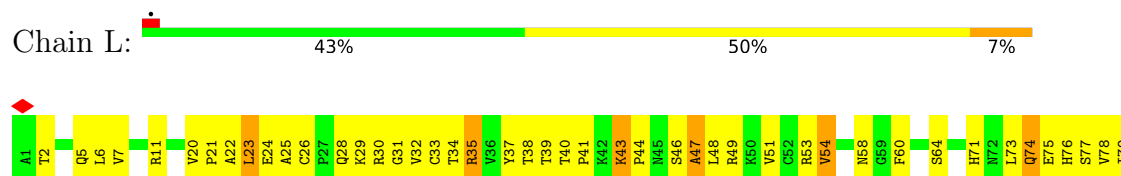
• Molecule 40: 30S ribosomal protein S10



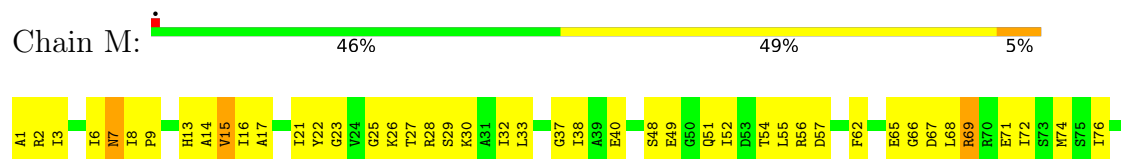
• Molecule 41: 30S ribosomal protein S11



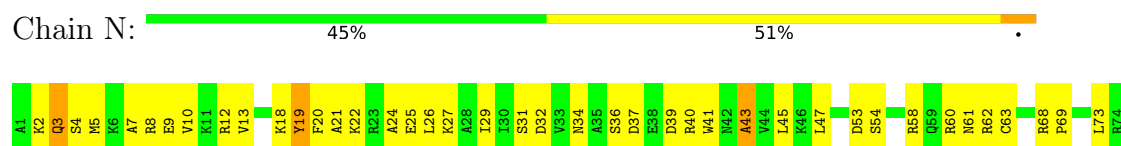
• Molecule 42: 30S ribosomal protein S12



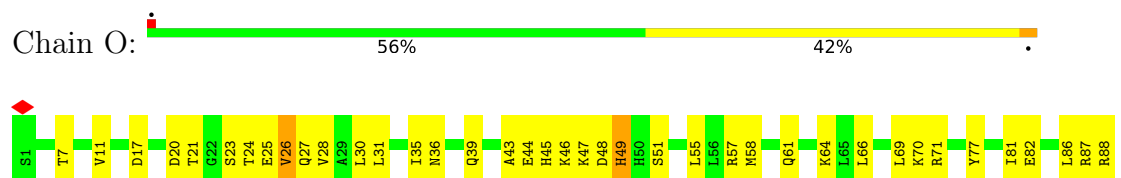
- Molecule 43: 30S ribosomal protein S13



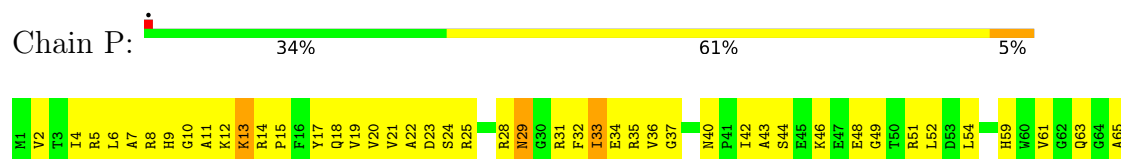
- Molecule 44: 30S ribosomal protein S14



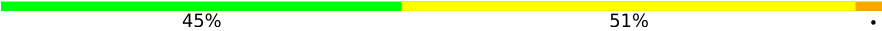
- Molecule 45: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S16



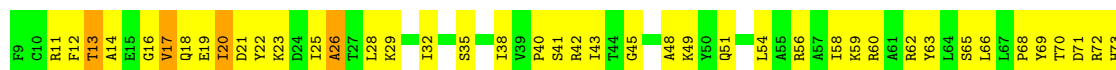
- Molecule 47: 30S ribosomal protein S17

Chain Q: 



- Molecule 48: 30S ribosomal protein S18

Chain R: 

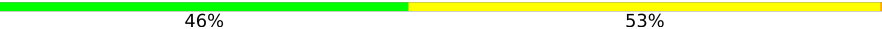


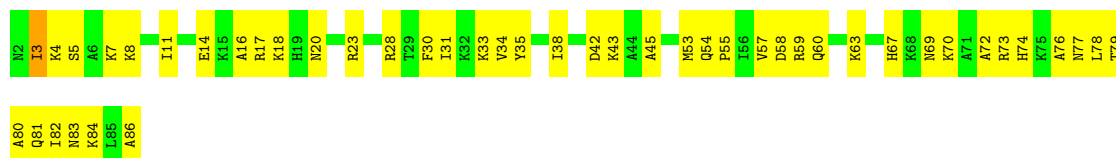
- Molecule 49: 30S ribosomal protein S19

Chain S: 



- Molecule 50: 30S ribosomal protein S20

Chain T: 



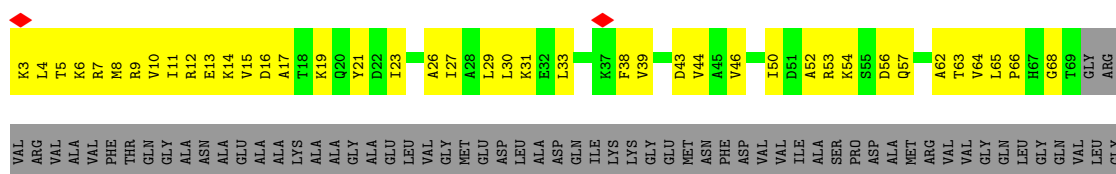
- Molecule 51: 30S ribosomal protein S21

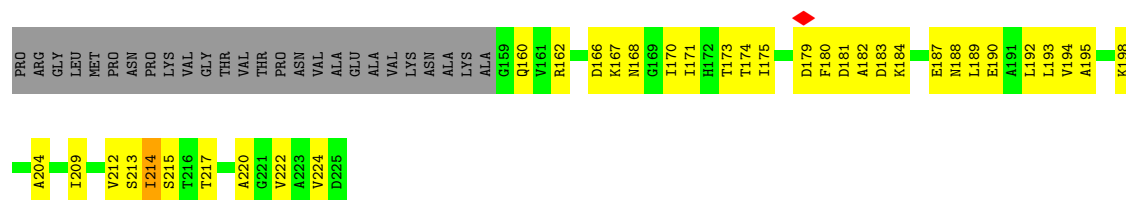
Chain U: 



- Molecule 52: 50S ribosomal protein L1

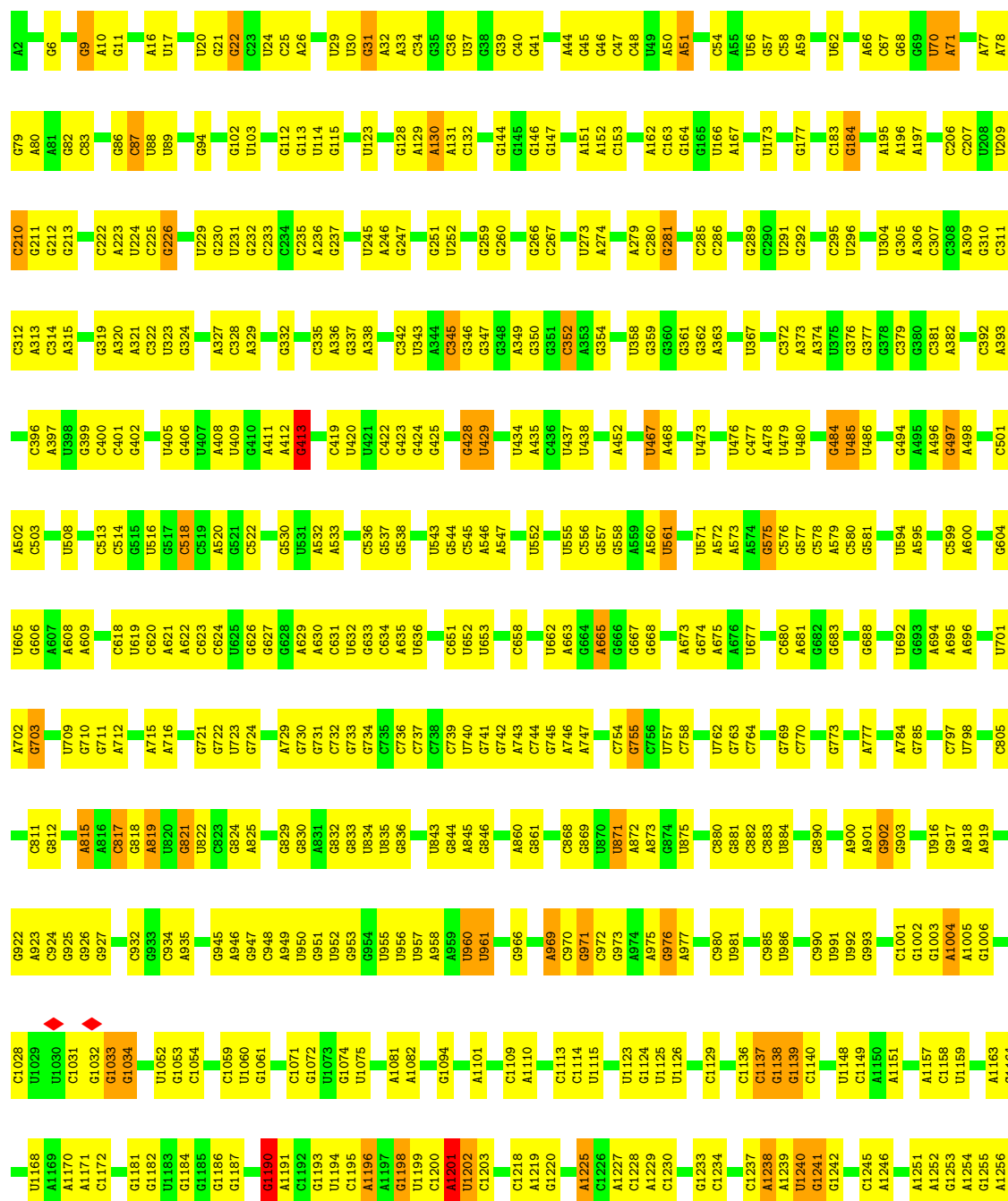
Chain 03: 





# Molecule 53: 16S ribosomal RNA

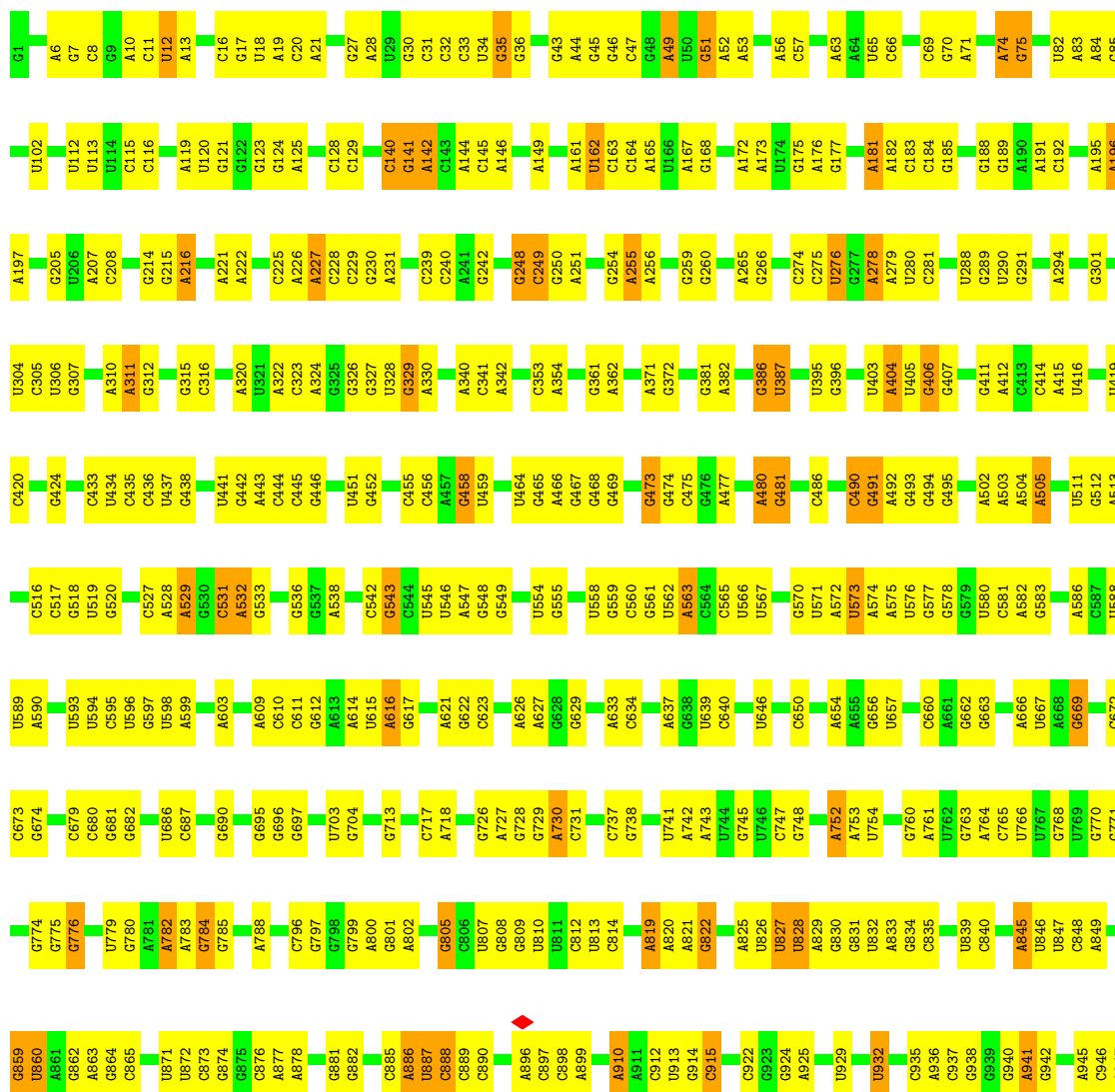
Chain A: 57% 38%





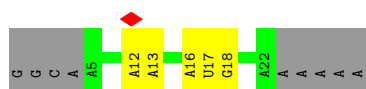
• Molecule 54: 23S ribosomal RNA

Chain 01: 54% 41% 5%



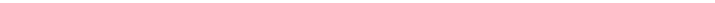
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C948  | G949  | C950  | C951  | G952  | G953  | G954  | G955  | G956  | C961  | G962  | C968  | G969  | G970  | G971  | A972  | A973  | G974  | A975  | A980  | A981  | G982  | A983  | A984  | G989  | C995  | A996  | G997  | A1001 | G1002 | C1007 | U1012 | C1013 | U1018 | U1019 | A1020 | A1021 | G1022 | U1023 | G1026 | A1027 | A1032 | U1033 | G1034 | U1035 | G1036 | G1037 | G1038 | A1039 |       |       |       |       |       |       |       |       |       |       |
| C1045 | A1046 | G1047 | C1053 | A1054 | G1055 | G1056 | G1059 | U1060 | U1061 | G1062 | G1063 | C1064 | U1065 | U1066 | A1067 | A1067 | A1067 | A1070 | G1071 | C1075 | U1076 | A1077 | U1078 | C1079 | A1080 | U1083 | A1084 | A1085 | A1088 | C1092 | G1093 | U1097 | A1098 | U1101 | C1102 | A1103 | C1104 | U1105 | G1106 | G1110 | A1111 | G1112 | U1113 | G1122 | A1128 | A1129 | U1130 | G1131 | U1132 |       |       |       |       |       |       |       |       |       |
| A1133 | A1134 | C1135 | G1138 | A1139 | C1140 | G954  | A1141 | A1142 | A1143 | G1149 | C1150 | C1153 | A1154 | A1155 | A1156 | A1157 | C1161 | G1162 | U1174 | A1175 | U1176 | C1177 | C1178 | G1179 | U1180 | U1181 | G1182 | U1183 | U1184 | G1185 | G1186 | G1187 | U1188 | A1189 | G1190 | G1191 | C1196 | G1197 | U1201 | G1202 | U1203 | A1204 | A1205 | U1209 | G1210 | C1211 | A1212 | A1213 | U1219 | U1130 | G1131 | U1132 |       |       |       |       |       |       |
| G1225 | G1236 | G1237 | A1237 | G1238 | C1243 | C1251 | G1252 | A1253 | U1344 | G1345 | G1346 | A1347 | C1348 | C1349 | C1350 | C1351 | U1352 | A1353 | A1354 | G1355 | G1356 | C1357 | G1358 | G1361 | C1362 | C1363 | C1364 | A1365 | A1366 | A1367 | G1368 | G1369 | C1370 | C1289 | G1371 | C1290 | C1297 | G1298 | G1299 | A1300 | A1301 | A1302 | U1313 | U1316 | G1317 | U1318 | A1319 | C1320 | A1321 | U1396 | U1397 | U1399 | A1395 | A1396 | U1397 | U1409 | G1410 | U1415 |
| G1416 | C1417 | G1418 | A1419 | A1420 | G1421 | G1422 | G1423 | G1424 | G1425 | G1430 | A1431 | G1432 | A1433 | A1434 | G1435 | G1436 | C1437 | U1438 | A1439 | U1440 | G1441 | U1442 | C1447 | G1448 | G1449 | C1450 | C1451 | C1454 | U1458 | G1459 | U1460 | C1461 | G1475 | U1476 | G1482 | A1490 | G1491 | C1498 | G1501 | A1502 | U1506 | C1507 | A1508 | A1509 | G1510 | A1515 | G1516 | U1517 |       |       |       |       |       |       |       |       |       |       |
| G1524 | A1525 | C1526 | G1527 | A1528 | G1529 | C1533 | U1534 | A1535 | C1536 | G1537 | G1538 | U1539 | A1540 | C1541 | U1542 | G1543 | A1544 | A1545 | A1548 | A1549 | G1555 | C1558 | U1559 | G1560 | C1561 | U1562 | U1563 | C1564 | G1565 | A1566 | A1569 | A1570 | A1571 | A1572 | G1581 | U1584 | C1585 | A1586 | G1587 | U1594 | C1595 | A1596 | A1597 | A1598 | U1599 | A1603 | A1608 | A1609 |       |       |       |       |       |       |       |       |       |       |
| A1610 | C1611 | C1612 | G1613 | A1614 | C1615 | A1616 | C1625 | A1626 | G1627 | G1628 | A1637 | C1638 | G1642 | G1643 | C1644 | G1645 | U1647 | U1648 | G1651 | A1652 | G1653 | A1654 | A1655 | C1656 | U1657 | C1658 | A1664 | A1665 | G1666 | A1667 | A1668 | A1669 | A1672 | G1673 | G1674 | C1675 | A1676 | A1677 | A1678 | A1679 | U1680 | G1681 | C1686 | G1687 | A1697 | A1698 | G1699 | C1704 | A1705 |       |       |       |       |       |       |       |       |       |
| G1715 | U1720 | G1721 | U1729 | C1730 | U1736 | A1737 | G1738 | A1749 | G1750 | G1753 | U1758 | A1759 | C1760 | C1764 | G1770 | C1771 | A1772 | A1773 | C1774 | U1775 | G1776 | U1779 | A1780 | U1781 | U1784 | A1785 | A1786 | A1787 | C1788 | A1789 | C1790 | A1791 | A1794 | C1795 | U1796 | G1797 | U1798 | G1799 | C1800 | A1801 | A1802 | A1803 | C1804 | A1805 | C1806 | A1807 | A1808 |       |       |       |       |       |       |       |       |       |       |       |
| A1809 | A1810 | U1811 | U1812 | G1813 | C1816 | A1817 | U1818 | A1819 | U1820 | U1825 | G1826 | U1827 | G1828 | C1833 | C1844 | G1845 | U1856 | G1857 | A1871 | A1872 | G1873 | U1883 | G1884 | A1885 | A1900 | A1901 | G1902 | G1903 | C1904 | G1905 | G1906 | G1907 | A1912 | A1913 | C1914 | U1917 | A1918 | G1929 | U1930 | U1931 | A1932 | C1933 | G1934 | U1935 | A1936 |       |       |       |       |       |       |       |       |       |       |       |       |       |
| A1937 | A1938 | U1943 | U1944 | G1949 | U1950 | U1951 | A1952 | A1953 | G1954 | U1955 | U1956 | C1961 | C1962 | U1963 | G1964 | A1965 | A1966 | C1967 | A1970 | U1971 | G1972 | G1973 | A1978 | U1979 | G1980 | G1983 | G1992 | U1993 | C1996 | C1997 | A1998 | C1999 | C2000 | C2001 | G2010 | U2011 | G2012 | A2015 | A2019 | A2020 | C2021 | U2022 | U2023 | G2024 | C2025 | U2026 | G2027 |       |       |       |       |       |       |       |       |       |       |       |
| A2030 | A2031 | U2034 | G2035 | C2036 | A2037 | G2038 | U2039 | G2040 | U2041 | A2042 | C2043 | C2044 | C2045 | G2049 | C2050 | A2051 | A2052 | G2053 | A2054 | C2055 | G2056 | A2060 | G2061 | A2062 | C2065 | C2066 | C2067 | U2068 | G2069 | A2070 | A2071 | C2072 | C2078 | U2079 | A2080 | U2081 | A2082 | G2083 | U2086 | G2087 | A2088 | C2096 | A2097 | U2098 | C2104 | U2105 | U2106 | G2110 | U2111 |       |       |       |       |       |       |       |       |       |
| G2112 | U2113 | U2118 | A2119 | G2120 | G2121 | U2122 | G2123 | G2124 | G2125 | A2126 | G2127 | G2128 | C2129 | U2130 | U2131 | U2132 | U2133 | A2134 | U2139 | G2140 | G2141 | G2144 | C2145 | C2146 | A2147 | U2151 | U2155 | A2156 | G2157 | A2158 | G2159 | G2162 | A2163 | C2164 | A2171 | U2172 | C2173 | C2175 | A2176 | C2177 | U2180 | A2183 | A2184 | G2187 | U2188 | U2189 | G2190 | U2191 |       |       |       |       |       |       |       |       |       |       |
| U2194 | U2195 | C2196 | A2197 | A2198 | U2203 | G2204 | A2205 | C2208 | G2209 | U2210 | A2211 | A2212 | U2213 | C2214 | C2215 | G2216 | G2224 | A2225 | G2230 | U2231 | C2232 | U2236 | G2237 | G2238 | G2239 | U2240 | A2241 | G2242 | U2243 | U2244 | U2245 | G2246 | A2247 | C2248 | U2249 | G2250 | U2257 | C2258 | U2262 | C2263 | C2264 | U2265 | A2266 | A2267 | A2268 | G2269 | A2270 | G2271 | G2276 | G2277 |       |       |       |       |       |       |       |       |

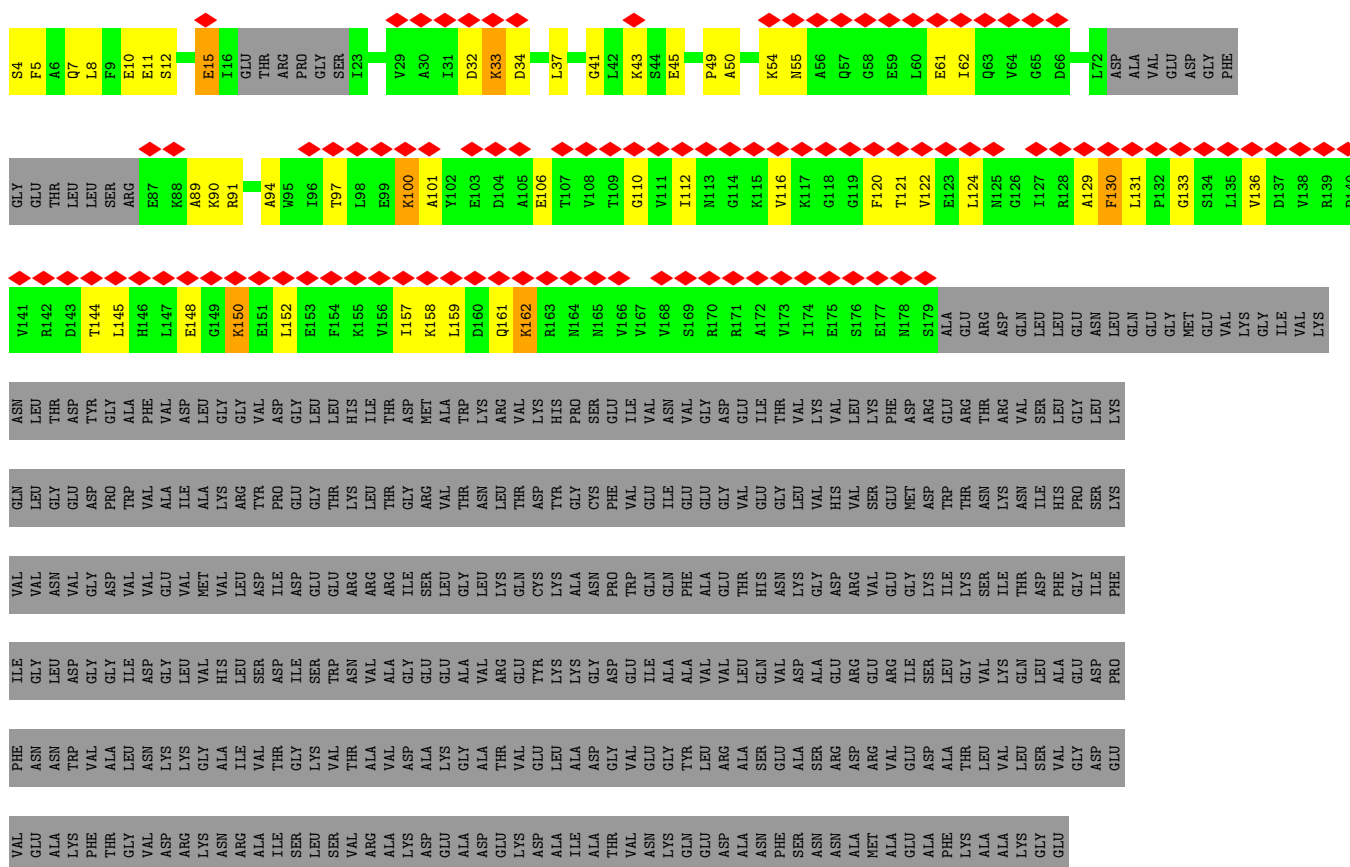




Chain Y:  63% 26% 9%



Chain Z: 



## 4 Experimental information

| Property                             | Value                                                                                                                | Source    |
|--------------------------------------|----------------------------------------------------------------------------------------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                                                                                                      | Depositor |
| Imposed symmetry                     | POINT, C1                                                                                                            | Depositor |
| Number of particles used             | 10289                                                                                                                | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                                                                                                    | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND3 was used to determine CTF values. FREALIGN applied CTF correction. | Depositor |
| Microscope                           | FEI TITAN KRIOS                                                                                                      | Depositor |
| Voltage (kV)                         | 300                                                                                                                  | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.0                                                                                                                  | Depositor |
| Minimum defocus (nm)                 | 500                                                                                                                  | Depositor |
| Maximum defocus (nm)                 | 5000                                                                                                                 | Depositor |
| Magnification                        | 60976                                                                                                                | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)                                                                                            | Depositor |
| Maximum map value                    | 0.062                                                                                                                | Depositor |
| Minimum map value                    | -0.023                                                                                                               | Depositor |
| Average map value                    | -0.001                                                                                                               | Depositor |
| Map value standard deviation         | 0.005                                                                                                                | Depositor |
| Recommended contour level            | 0.01                                                                                                                 | Depositor |
| Map size (Å)                         | 393.6, 393.6, 393.6                                                                                                  | wwPDB     |
| Map dimensions                       | 480, 480, 480                                                                                                        | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                                                                                                     | wwPDB     |
| Pixel spacing (Å)                    | 0.82, 0.82, 0.82                                                                                                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$    |
| 1   | 04    | 0.30         | 0/2122      | 0.91        | 5/2852 (0.2%)  |
| 2   | 05    | 0.29         | 0/1586      | 0.81        | 1/2134 (0.0%)  |
| 3   | 06    | 0.29         | 0/1571      | 0.81        | 3/2113 (0.1%)  |
| 4   | 07    | 0.29         | 0/1435      | 0.88        | 2/1926 (0.1%)  |
| 5   | 08    | 0.30         | 0/1343      | 0.85        | 3/1816 (0.2%)  |
| 6   | 09    | 0.30         | 0/1122      | 0.90        | 5/1515 (0.3%)  |
| 7   | 10    | 0.33         | 0/1002      | 1.02        | 11/1350 (0.8%) |
| 8   | 11    | 0.35         | 0/1046      | 0.93        | 1/1410 (0.1%)  |
| 9   | 12    | 0.29         | 0/1152      | 0.80        | 0/1551         |
| 10  | 13    | 0.28         | 0/948       | 0.89        | 2/1268 (0.2%)  |
| 11  | 14    | 0.29         | 0/1054      | 0.83        | 1/1403 (0.1%)  |
| 12  | 15    | 0.27         | 0/1093      | 0.82        | 3/1460 (0.2%)  |
| 13  | 16    | 0.29         | 0/974       | 0.82        | 0/1301         |
| 14  | 17    | 0.28         | 0/902       | 0.73        | 0/1209         |
| 15  | 18    | 0.28         | 0/929       | 0.81        | 2/1242 (0.2%)  |
| 16  | 19    | 0.29         | 0/960       | 0.82        | 1/1278 (0.1%)  |
| 17  | 20    | 0.28         | 0/829       | 0.87        | 3/1107 (0.3%)  |
| 18  | 21    | 0.28         | 0/864       | 0.84        | 1/1156 (0.1%)  |
| 19  | 22    | 0.27         | 0/745       | 0.78        | 0/994          |
| 20  | 23    | 0.27         | 0/788       | 0.77        | 1/1051 (0.1%)  |
| 21  | 24    | 0.28         | 0/766       | 0.81        | 0/1025         |
| 22  | 25    | 0.28         | 0/582       | 0.84        | 0/769          |
| 23  | 26    | 0.28         | 0/635       | 0.79        | 0/848          |
| 24  | 27    | 0.27         | 0/510       | 0.73        | 0/677          |
| 25  | 28    | 0.28         | 0/453       | 0.84        | 0/605          |
| 26  | 29    | 0.29         | 0/532       | 0.84        | 2/709 (0.3%)   |
| 27  | 30    | 0.28         | 0/450       | 0.82        | 1/599 (0.2%)   |
| 28  | 31    | 0.30         | 0/417       | 0.78        | 0/554          |
| 29  | 32    | 0.31         | 0/380       | 0.82        | 0/498          |
| 30  | 33    | 0.29         | 0/513       | 0.78        | 2/676 (0.3%)   |
| 31  | 34    | 0.33         | 0/303       | 0.97        | 2/397 (0.5%)   |
| 32  | B     | 0.29         | 0/1788      | 0.88        | 2/2408 (0.1%)  |

| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 33  | C     | 0.30         | 0/1652   | 0.88        | 7/2225 (0.3%)     |
| 34  | D     | 0.28         | 0/1665   | 0.85        | 2/2227 (0.1%)     |
| 35  | E     | 0.30         | 0/1170   | 0.87        | 3/1573 (0.2%)     |
| 36  | F     | 0.42         | 0/1048   | 0.93        | 5/1413 (0.4%)     |
| 37  | G     | 0.28         | 0/1196   | 0.90        | 5/1602 (0.3%)     |
| 38  | H     | 0.29         | 0/989    | 0.88        | 3/1326 (0.2%)     |
| 39  | I     | 0.29         | 0/1034   | 0.85        | 3/1375 (0.2%)     |
| 40  | J     | 0.31         | 0/797    | 0.91        | 4/1077 (0.4%)     |
| 41  | K     | 0.31         | 0/886    | 0.94        | 3/1195 (0.3%)     |
| 42  | L     | 0.31         | 0/969    | 0.99        | 5/1300 (0.4%)     |
| 43  | M     | 0.29         | 0/893    | 0.82        | 2/1193 (0.2%)     |
| 44  | N     | 0.28         | 0/817    | 0.76        | 0/1088            |
| 45  | O     | 0.28         | 0/722    | 0.75        | 1/964 (0.1%)      |
| 46  | P     | 0.30         | 0/659    | 0.86        | 3/884 (0.3%)      |
| 47  | Q     | 0.30         | 0/658    | 0.87        | 3/881 (0.3%)      |
| 48  | R     | 0.32         | 0/545    | 0.85        | 2/731 (0.3%)      |
| 49  | S     | 0.30         | 0/653    | 0.87        | 1/877 (0.1%)      |
| 50  | T     | 0.30         | 0/671    | 0.87        | 2/888 (0.2%)      |
| 51  | U     | 0.31         | 0/551    | 0.89        | 2/728 (0.3%)      |
| 52  | 03    | 0.30         | 0/1034   | 0.84        | 0/1387            |
| 53  | A     | 0.42         | 0/36963  | 0.48        | 3/57662 (0.0%)    |
| 54  | 01    | 0.41         | 0/69796  | 0.49        | 2/108888 (0.0%)   |
| 55  | 02    | 0.42         | 0/2872   | 0.47        | 0/4479            |
| 56  | W     | 0.41         | 0/1832   | 0.44        | 0/2855            |
| 56  | X     | 0.41         | 0/1832   | 0.49        | 0/2855            |
| 57  | V     | 0.42         | 0/436    | 0.48        | 0/679             |
| 58  | Y     | 0.43         | 0/1812   | 0.49        | 1/2823 (0.0%)     |
| 59  | Z     | 0.51         | 0/1215   | 0.78        | 1/1635 (0.1%)     |
| All | All   | 0.38         | 0/165161 | 0.61        | 117/246711 (0.0%) |

There are no bond length outliers.

All (117) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | 08    | 10  | VAL  | N-CA-C | 9.06  | 118.06      | 107.73   |
| 42  | L     | 114 | SER  | N-CA-C | -8.64 | 101.83      | 111.07   |
| 37  | G     | 5   | VAL  | N-CA-C | -7.70 | 105.06      | 112.29   |
| 7   | 10    | 117 | LEU  | N-CA-C | 7.69  | 120.23      | 109.15   |
| 37  | G     | 80  | GLY  | N-CA-C | -7.33 | 105.13      | 114.37   |
| 7   | 10    | 119 | PRO  | N-CA-C | -7.28 | 104.07      | 114.18   |
| 50  | T     | 5   | SER  | N-CA-C | -7.23 | 104.33      | 113.01   |
| 7   | 10    | 30  | SER  | N-CA-C | -7.06 | 104.79      | 113.41   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 40  | J     | 30   | LYS  | N-CA-C      | -6.93 | 104.08      | 112.54   |
| 1   | 04    | 13   | ARG  | N-CA-C      | 6.93  | 119.43      | 111.11   |
| 42  | L     | 93   | ARG  | N-CA-C      | 6.88  | 120.63      | 112.93   |
| 10  | 13    | 32   | TYR  | N-CA-C      | 6.58  | 120.25      | 110.52   |
| 41  | K     | 117  | HIS  | N-CA-C      | -6.55 | 105.16      | 112.57   |
| 8   | 11    | 111  | THR  | N-CA-C      | -6.48 | 104.30      | 111.82   |
| 10  | 13    | 41   | ILE  | N-CA-C      | 6.44  | 116.67      | 108.82   |
| 26  | 29    | 45   | THR  | N-CA-C      | -6.43 | 105.59      | 113.50   |
| 53  | A     | 1190 | G    | C2'-C3'-O3' | 6.35  | 119.02      | 109.50   |
| 47  | Q     | 33   | TYR  | N-CA-C      | 6.33  | 120.11      | 112.38   |
| 33  | C     | 14   | VAL  | N-CA-C      | 6.30  | 116.98      | 110.36   |
| 42  | L     | 115  | LYS  | N-CA-C      | -6.26 | 101.67      | 110.50   |
| 16  | 19    | 49   | ARG  | N-CA-C      | -6.26 | 104.90      | 112.54   |
| 43  | M     | 112  | ARG  | N-CA-C      | 6.25  | 118.36      | 108.67   |
| 7   | 10    | 42   | ARG  | N-CA-C      | -6.20 | 105.20      | 112.89   |
| 51  | U     | 17   | ARG  | N-CA-C      | -6.15 | 106.38      | 114.31   |
| 17  | 20    | 50   | GLY  | N-CA-C      | -6.10 | 98.73       | 113.18   |
| 3   | 06    | 178  | VAL  | N-CA-C      | 6.09  | 116.21      | 110.30   |
| 20  | 23    | 76   | THR  | N-CA-C      | -6.08 | 105.83      | 113.18   |
| 43  | M     | 105  | ALA  | N-CA-C      | -6.08 | 104.47      | 113.40   |
| 47  | Q     | 51   | GLU  | N-CA-C      | -6.06 | 105.18      | 113.30   |
| 27  | 30    | 18   | HIS  | N-CA-C      | 6.05  | 117.87      | 111.28   |
| 41  | K     | 70   | ALA  | N-CA-C      | -5.97 | 105.09      | 112.38   |
| 40  | J     | 59   | LYS  | N-CA-C      | -5.97 | 105.96      | 113.18   |
| 33  | C     | 143  | LEU  | N-CA-C      | -5.96 | 105.65      | 113.17   |
| 15  | 18    | 33   | GLU  | N-CA-C      | -5.95 | 105.84      | 112.57   |
| 3   | 06    | 6    | LYS  | N-CA-C      | 5.94  | 117.45      | 110.97   |
| 59  | Z     | 15   | GLU  | N-CA-C      | -5.91 | 105.65      | 112.92   |
| 38  | H     | 118  | ALA  | N-CA-C      | -5.90 | 106.08      | 113.28   |
| 6   | 09    | 117  | LEU  | CA-C-N      | 5.89  | 127.20      | 119.84   |
| 6   | 09    | 117  | LEU  | C-N-CA      | 5.89  | 127.20      | 119.84   |
| 46  | P     | 79   | ASN  | CB-CA-C     | -5.88 | 108.79      | 115.79   |
| 38  | H     | 76   | ARG  | N-CA-C      | -5.87 | 100.96      | 109.59   |
| 35  | E     | 110  | MET  | N-CA-C      | -5.85 | 104.49      | 111.69   |
| 26  | 29    | 54   | GLY  | N-CA-C      | 5.77  | 122.38      | 112.51   |
| 31  | 34    | 30   | GLU  | CA-C-N      | 5.76  | 125.88      | 119.32   |
| 31  | 34    | 30   | GLU  | C-N-CA      | 5.76  | 125.88      | 119.32   |
| 6   | 09    | 71   | LYS  | N-CA-C      | 5.75  | 118.33      | 111.71   |
| 15  | 18    | 11   | GLN  | N-CA-C      | -5.74 | 106.90      | 114.31   |
| 40  | J     | 27   | GLU  | N-CA-C      | -5.72 | 104.95      | 111.07   |
| 32  | B     | 124  | THR  | N-CA-C      | -5.70 | 105.20      | 111.82   |
| 1   | 04    | 225  | ASN  | CA-C-N      | 5.67  | 126.92      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 04    | 225  | ASN  | C-N-CA      | 5.67  | 126.92      | 119.84   |
| 12  | 15    | 118  | LYS  | N-CA-C      | -5.58 | 105.27      | 111.36   |
| 33  | C     | 5    | HIS  | CA-C-N      | 5.55  | 126.78      | 119.84   |
| 33  | C     | 5    | HIS  | C-N-CA      | 5.55  | 126.78      | 119.84   |
| 37  | G     | 76   | SER  | N-CA-C      | 5.55  | 117.57      | 108.52   |
| 11  | 14    | 63   | LYS  | N-CA-C      | -5.55 | 102.55      | 110.59   |
| 5   | 08    | 47   | ASN  | N-CA-C      | -5.54 | 105.24      | 111.28   |
| 39  | I     | 92   | SER  | N-CA-C      | -5.54 | 105.14      | 112.34   |
| 42  | L     | 54   | VAL  | N-CA-C      | 5.54  | 116.71      | 108.46   |
| 36  | F     | 18   | VAL  | CB-CA-C     | -5.53 | 108.45      | 113.70   |
| 46  | P     | 61   | VAL  | N-CA-C      | -5.51 | 104.20      | 111.09   |
| 6   | 09    | 70   | GLU  | N-CA-C      | 5.49  | 117.12      | 111.03   |
| 1   | 04    | 66   | PHE  | N-CA-C      | -5.47 | 106.73      | 113.41   |
| 7   | 10    | 118  | ILE  | CA-C-N      | -5.47 | 114.11      | 119.64   |
| 7   | 10    | 118  | ILE  | C-N-CA      | -5.47 | 114.11      | 119.64   |
| 40  | J     | 26   | VAL  | N-CA-C      | -5.45 | 105.06      | 111.00   |
| 54  | 01    | 1064 | C    | N1-C1'-C2'  | 5.45  | 120.17      | 112.00   |
| 7   | 10    | 57   | ASN  | N-CA-C      | -5.44 | 105.34      | 112.41   |
| 36  | F     | 49   | TYR  | CA-C-N      | 5.42  | 126.62      | 119.84   |
| 36  | F     | 49   | TYR  | C-N-CA      | 5.42  | 126.62      | 119.84   |
| 45  | O     | 43   | ALA  | N-CA-C      | -5.41 | 104.79      | 111.33   |
| 37  | G     | 129  | ASN  | N-CA-C      | 5.41  | 118.65      | 111.30   |
| 33  | C     | 67   | ILE  | N-CA-C      | 5.40  | 115.89      | 108.12   |
| 7   | 10    | 43   | LYS  | N-CA-C      | -5.39 | 105.97      | 112.54   |
| 54  | 01    | 1020 | A    | C2'-C3'-O3' | 5.33  | 117.49      | 109.50   |
| 7   | 10    | 54   | VAL  | N-CA-C      | -5.32 | 106.23      | 111.77   |
| 51  | U     | 66   | ARG  | N-CA-C      | -5.30 | 104.71      | 110.91   |
| 1   | 04    | 265  | PHE  | N-CA-C      | 5.29  | 116.90      | 111.03   |
| 18  | 21    | 42   | LYS  | N-CA-C      | -5.27 | 105.61      | 111.36   |
| 34  | D     | 44   | LYS  | CA-C-N      | 5.26  | 125.51      | 119.83   |
| 34  | D     | 44   | LYS  | C-N-CA      | 5.26  | 125.51      | 119.83   |
| 58  | Y     | 63   | G    | C2'-C3'-O3' | 5.26  | 121.59      | 113.70   |
| 17  | 20    | 13   | ARG  | N-CA-C      | -5.25 | 101.59      | 109.15   |
| 3   | 06    | 41   | GLN  | N-CA-C      | -5.25 | 106.83      | 113.18   |
| 36  | F     | 66   | ALA  | N-CA-C      | 5.24  | 112.73      | 108.07   |
| 5   | 08    | 139  | VAL  | N-CA-C      | 5.24  | 115.45      | 110.42   |
| 46  | P     | 76   | LYS  | N-CA-C      | -5.23 | 106.04      | 112.90   |
| 50  | T     | 7    | LYS  | N-CA-C      | -5.23 | 106.16      | 112.54   |
| 30  | 33    | 61   | LEU  | CA-C-N      | 5.22  | 126.37      | 119.84   |
| 30  | 33    | 61   | LEU  | C-N-CA      | 5.22  | 126.37      | 119.84   |
| 2   | 05    | 102  | ALA  | N-CA-C      | -5.22 | 106.75      | 113.01   |
| 6   | 09    | 63   | ALA  | N-CA-C      | -5.21 | 105.60      | 111.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32  | B     | 112  | ARG  | N-CA-C      | -5.21 | 105.68      | 111.36   |
| 48  | R     | 66   | LEU  | N-CA-C      | -5.19 | 106.63      | 113.12   |
| 17  | 20    | 75   | VAL  | N-CA-C      | 5.17  | 114.95      | 106.72   |
| 53  | A     | 1201 | A    | C2'-C3'-O3' | 5.17  | 117.26      | 109.50   |
| 39  | I     | 6    | TYR  | N-CA-C      | 5.17  | 118.02      | 109.85   |
| 41  | K     | 69   | CYS  | N-CA-C      | -5.17 | 105.72      | 112.23   |
| 48  | R     | 28   | LEU  | N-CA-C      | 5.16  | 116.60      | 110.97   |
| 7   | 10    | 58   | THR  | N-CA-C      | 5.16  | 121.78      | 110.80   |
| 12  | 15    | 25   | ASP  | N-CA-C      | 5.15  | 118.13      | 110.14   |
| 35  | E     | 131  | ASN  | CA-C-N      | 5.15  | 126.28      | 119.84   |
| 35  | E     | 131  | ASN  | C-N-CA      | 5.15  | 126.28      | 119.84   |
| 38  | H     | 99   | GLY  | N-CA-C      | -5.14 | 102.52      | 111.62   |
| 47  | Q     | 15   | LYS  | N-CA-C      | 5.14  | 121.74      | 110.80   |
| 36  | F     | 116  | PHE  | N-CA-C      | -5.13 | 105.76      | 112.23   |
| 33  | C     | 98   | ALA  | N-CA-C      | 5.13  | 117.76      | 108.69   |
| 39  | I     | 119  | LYS  | N-CA-C      | 5.12  | 116.25      | 107.28   |
| 37  | G     | 40   | SER  | N-CA-C      | -5.09 | 105.73      | 111.28   |
| 12  | 15    | 107  | GLY  | N-CA-C      | -5.07 | 107.69      | 116.01   |
| 42  | L     | 74   | GLN  | N-CA-C      | 5.06  | 116.55      | 107.80   |
| 7   | 10    | 53   | ARG  | N-CA-C      | 5.06  | 117.48      | 109.24   |
| 53  | A     | 413  | G    | N9-C1'-C2'  | 5.05  | 119.57      | 112.00   |
| 33  | C     | 106  | ARG  | N-CA-C      | 5.04  | 118.69      | 112.54   |
| 49  | S     | 57   | VAL  | N-CA-C      | 5.03  | 113.98      | 108.05   |
| 4   | 07    | 174  | PHE  | CA-C-N      | 5.00  | 126.10      | 119.84   |
| 4   | 07    | 174  | PHE  | C-N-CA      | 5.00  | 126.10      | 119.84   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 04    | 2083  | 0        | 2157     | 134     | 0            |
| 2   | 05    | 1565  | 0        | 1616     | 82      | 0            |
| 3   | 06    | 1552  | 0        | 1619     | 105     | 0            |
| 4   | 07    | 1411  | 0        | 1447     | 105     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | 08    | 1323  | 0        | 1374     | 73      | 0            |
| 6   | 09    | 1111  | 0        | 1148     | 79      | 0            |
| 7   | 10    | 989   | 0        | 1025     | 85      | 0            |
| 8   | 11    | 1032  | 0        | 1088     | 87      | 0            |
| 9   | 12    | 1129  | 0        | 1162     | 83      | 0            |
| 10  | 13    | 939   | 0        | 1012     | 59      | 0            |
| 11  | 14    | 1045  | 0        | 1117     | 69      | 0            |
| 12  | 15    | 1074  | 0        | 1157     | 68      | 0            |
| 13  | 16    | 961   | 0        | 1000     | 71      | 0            |
| 14  | 17    | 892   | 0        | 923      | 53      | 0            |
| 15  | 18    | 917   | 0        | 965      | 73      | 0            |
| 16  | 19    | 947   | 0        | 1022     | 71      | 0            |
| 17  | 20    | 816   | 0        | 839      | 56      | 0            |
| 18  | 21    | 857   | 0        | 922      | 65      | 0            |
| 19  | 22    | 739   | 0        | 807      | 39      | 0            |
| 20  | 23    | 780   | 0        | 834      | 40      | 0            |
| 21  | 24    | 753   | 0        | 780      | 31      | 0            |
| 22  | 25    | 575   | 0        | 592      | 23      | 0            |
| 23  | 26    | 625   | 0        | 655      | 22      | 0            |
| 24  | 27    | 509   | 0        | 543      | 30      | 0            |
| 25  | 28    | 449   | 0        | 491      | 32      | 0            |
| 26  | 29    | 523   | 0        | 524      | 24      | 0            |
| 27  | 30    | 444   | 0        | 461      | 44      | 0            |
| 28  | 31    | 410   | 0        | 440      | 21      | 0            |
| 29  | 32    | 377   | 0        | 418      | 21      | 0            |
| 30  | 33    | 504   | 0        | 574      | 20      | 0            |
| 31  | 34    | 302   | 0        | 343      | 22      | 0            |
| 32  | B     | 1757  | 0        | 1787     | 84      | 0            |
| 33  | C     | 1625  | 0        | 1699     | 94      | 0            |
| 34  | D     | 1643  | 0        | 1710     | 128     | 0            |
| 35  | E     | 1157  | 0        | 1199     | 105     | 0            |
| 36  | F     | 1028  | 0        | 1002     | 66      | 0            |
| 37  | G     | 1182  | 0        | 1240     | 72      | 0            |
| 38  | H     | 979   | 0        | 1034     | 69      | 0            |
| 39  | I     | 1022  | 0        | 1070     | 76      | 0            |
| 40  | J     | 787   | 0        | 828      | 63      | 0            |
| 41  | K     | 870   | 0        | 878      | 69      | 0            |
| 42  | L     | 955   | 0        | 1019     | 75      | 0            |
| 43  | M     | 884   | 0        | 944      | 70      | 0            |
| 44  | N     | 805   | 0        | 847      | 61      | 0            |
| 45  | O     | 714   | 0        | 737      | 31      | 0            |
| 46  | P     | 649   | 0        | 666      | 67      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 47  | Q     | 649    | 0        | 691      | 47      | 0            |
| 48  | R     | 536    | 0        | 552      | 44      | 0            |
| 49  | S     | 638    | 0        | 665      | 35      | 0            |
| 50  | T     | 665    | 0        | 714      | 41      | 0            |
| 51  | U     | 545    | 0        | 579      | 65      | 0            |
| 52  | 03    | 1027   | 0        | 1092     | 68      | 0            |
| 53  | A     | 33012  | 0        | 16618    | 510     | 0            |
| 54  | 01    | 62317  | 0        | 31346    | 1011    | 0            |
| 55  | 02    | 2568   | 0        | 1303     | 47      | 0            |
| 56  | W     | 1640   | 0        | 836      | 12      | 0            |
| 56  | X     | 1640   | 0        | 837      | 19      | 0            |
| 57  | V     | 388    | 0        | 196      | 3       | 0            |
| 58  | Y     | 1622   | 0        | 821      | 17      | 0            |
| 59  | Z     | 1204   | 0        | 1221     | 61      | 0            |
| 60  | W     | 10     | 0        | 10       | 0       | 0            |
| All | All   | 152151 | 0        | 103196   | 4455    | 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 17.

All (4455) 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) |
|--------------------|-------------------|--------------------------|-------------------|
| 15:18:59:THR:HG22  | 15:18:72:VAL:HG12 | 1.33                     | 1.10              |
| 54:01:45:G:H5''    | 54:01:46:G:H5'    | 1.22                     | 1.09              |
| 14:17:29:HIS:HB3   | 14:17:36:TYR:HB2  | 1.37                     | 1.04              |
| 52:03:174:THR:HG21 | 54:01:2124:G:H4'  | 1.39                     | 1.04              |
| 43:M:97:ARG:HB2    | 43:M:99:GLN:HE22  | 1.23                     | 1.03              |
| 34:D:33:ILE:HG13   | 34:D:34:GLU:H     | 1.24                     | 1.02              |
| 54:01:275:C:H2'    | 54:01:276:U:H4'   | 1.41                     | 1.02              |
| 1:04:20:ASN:HD21   | 1:04:22:GLU:HB2   | 1.26                     | 1.01              |
| 56:X:13:C:H2'      | 56:X:14:A:H5''    | 1.38                     | 1.01              |
| 39:I:104:THR:HG22  | 39:I:106:ASP:H    | 1.26                     | 1.00              |
| 8:11:91:LYS:HB3    | 8:11:94:LYS:HB2   | 1.44                     | 0.99              |
| 53:A:484:G:H4'     | 53:A:485:U:H5''   | 1.44                     | 0.99              |
| 2:05:151:THR:HB    | 2:05:152:PRO:HD3  | 1.44                     | 0.98              |
| 6:09:72:ILE:HB     | 6:09:108:VAL:HG22 | 1.43                     | 0.98              |
| 39:I:20:ILE:HD11   | 39:I:60:LEU:HD22  | 1.43                     | 0.97              |
| 8:11:15:GLY:HA2    | 8:11:50:LYS:HB3   | 1.44                     | 0.97              |
| 53:A:1259:C:H3'    | 53:A:1260:G:H5''  | 1.47                     | 0.96              |
| 31:34:1:MET:HE2    | 31:34:36:ARG:HB3  | 1.46                     | 0.95              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:J:57:VAL:HG22   | 40:J:58:ASN:H      | 1.28                     | 0.95              |
| 33:C:59:PRO:HG2    | 33:C:62:SER:HB3    | 1.48                     | 0.95              |
| 55:02:3:C:H2'      | 55:02:4:C:H5''     | 1.45                     | 0.95              |
| 43:M:2:ARG:HE      | 43:M:8:ILE:HD11    | 1.31                     | 0.94              |
| 41:K:34:THR:HG22   | 41:K:40:ALA:HA     | 1.46                     | 0.94              |
| 37:G:12:LEU:HD11   | 39:I:49:GLN:HE22   | 1.32                     | 0.94              |
| 43:M:113:LYS:H     | 43:M:114:PRO:HD2   | 1.31                     | 0.93              |
| 54:01:2277:G:H2'   | 54:01:2278:A:H5''  | 1.51                     | 0.93              |
| 43:M:15:VAL:HG23   | 43:M:16:ILE:HD12   | 1.50                     | 0.92              |
| 32:B:202:ASN:HD21  | 32:B:205:ALA:HB2   | 1.34                     | 0.92              |
| 11:14:101:ILE:HG13 | 11:14:102:GLY:H    | 1.32                     | 0.91              |
| 35:E:133:ILE:HD12  | 35:E:133:ILE:H     | 1.32                     | 0.91              |
| 35:E:80:LEU:HD13   | 35:E:122:VAL:HG11  | 1.49                     | 0.91              |
| 49:S:27:LYS:HG2    | 49:S:28:LYS:H      | 1.34                     | 0.91              |
| 12:15:20:LEU:HD23  | 21:24:81:PRO:HG2   | 1.54                     | 0.90              |
| 47:Q:37:ILE:HD12   | 47:Q:39:ARG:HH21   | 1.37                     | 0.90              |
| 54:01:821:A:H5''   | 54:01:822:G:H5''   | 1.54                     | 0.89              |
| 24:27:2:LYS:HG3    | 24:27:3:ALA:H      | 1.36                     | 0.89              |
| 4:07:104:THR:HA    | 26:29:38:SER:HB3   | 1.52                     | 0.89              |
| 10:13:40:LYS:HE3   | 10:13:57:VAL:HG12  | 1.52                     | 0.89              |
| 25:28:4:ILE:HD11   | 25:28:56:VAL:HG23  | 1.55                     | 0.88              |
| 48:R:11:ARG:HD3    | 53:A:845:A:H4'     | 1.55                     | 0.88              |
| 1:04:16:VAL:HB     | 1:04:203:VAL:HG22  | 1.54                     | 0.88              |
| 46:P:48:GLU:HG3    | 46:P:49:GLY:H      | 1.39                     | 0.88              |
| 12:15:60:GLN:HE21  | 12:15:108:VAL:HG12 | 1.38                     | 0.88              |
| 32:B:202:ASN:HD21  | 32:B:205:ALA:CB    | 1.87                     | 0.88              |
| 20:23:33:VAL:HG13  | 20:23:66:VAL:HG22  | 1.56                     | 0.88              |
| 40:J:30:LYS:HA     | 40:J:34:ALA:HA     | 1.56                     | 0.88              |
| 37:G:12:LEU:HD12   | 37:G:13:PRO:HD2    | 1.53                     | 0.87              |
| 54:01:1664:A:H61   | 54:01:1996:C:H42   | 1.18                     | 0.87              |
| 1:04:20:ASN:ND2    | 1:04:22:GLU:HB2    | 1.90                     | 0.87              |
| 12:15:45:GLN:HE21  | 54:01:2485:G:H5''  | 1.39                     | 0.87              |
| 20:23:39:ASN:O     | 20:23:61:GLU:HA    | 1.75                     | 0.87              |
| 59:Z:162:LYS:N     | 59:Z:162:LYS:HE3   | 1.90                     | 0.87              |
| 35:E:76:ASN:HB2    | 35:E:81:GLN:NE2    | 1.89                     | 0.86              |
| 49:S:62:THR:HG22   | 49:S:63:ASP:H      | 1.40                     | 0.86              |
| 8:11:59:THR:HB     | 8:11:67:THR:HB     | 1.55                     | 0.86              |
| 35:E:93:VAL:HG13   | 35:E:110:MET:HE2   | 1.57                     | 0.86              |
| 56:X:47:U:H5''     | 56:X:48:C:H5'      | 1.58                     | 0.86              |
| 35:E:107:GLY:HA3   | 53:A:9:G:H5'       | 1.55                     | 0.86              |
| 6:09:73:ASN:ND2    | 6:09:76:GLU:HA     | 1.91                     | 0.86              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:25:36:GLN:NE2  | 22:25:39:THR:HA    | 1.90                     | 0.85              |
| 33:C:39:ARG:HG3   | 33:C:54:ILE:HD11   | 1.57                     | 0.85              |
| 34:D:56:GLU:HG2   | 34:D:198:LEU:HB2   | 1.58                     | 0.85              |
| 35:E:163:ILE:HD12 | 35:E:164:LEU:N     | 1.90                     | 0.85              |
| 40:J:6:ILE:HB     | 40:J:76:ILE:HB     | 1.56                     | 0.85              |
| 6:09:78:VAL:HG21  | 6:09:103:VAL:HG22  | 1.57                     | 0.85              |
| 11:14:14:LYS:HA   | 11:14:14:LYS:HE3   | 1.59                     | 0.85              |
| 44:N:8:ARG:HG2    | 44:N:12:ARG:HH12   | 1.40                     | 0.85              |
| 5:08:21:GLN:HE21  | 5:08:36:LEU:HB2    | 1.41                     | 0.85              |
| 9:12:81:ILE:HG13  | 9:12:82:GLY:H      | 1.39                     | 0.85              |
| 6:09:8:LYS:O      | 6:09:13:GLY:HA3    | 1.76                     | 0.84              |
| 14:17:51:ALA:HB3  | 14:17:78:VAL:HG22  | 1.59                     | 0.84              |
| 34:D:195:ASN:HD22 | 34:D:198:LEU:HG    | 1.43                     | 0.84              |
| 54:01:1020:A:H1'  | 54:01:1021:A:OP2   | 1.78                     | 0.84              |
| 47:Q:69:THR:HG22  | 47:Q:70:LYS:H      | 1.42                     | 0.84              |
| 1:04:47:ARG:HH21  | 54:01:774:G:H5''   | 1.41                     | 0.83              |
| 8:11:89:SER:HB3   | 54:01:1063:G:H2'   | 1.57                     | 0.83              |
| 2:05:33:ARG:HD3   | 2:05:73:VAL:HB     | 1.59                     | 0.83              |
| 7:10:27:VAL:HG23  | 7:10:110:ALA:HB1   | 1.59                     | 0.83              |
| 20:23:73:ASN:HD22 | 20:23:76:THR:H     | 1.22                     | 0.83              |
| 8:11:27:LEU:HD12  | 8:11:28:GLY:N      | 1.93                     | 0.83              |
| 37:G:129:ASN:HA   | 37:G:134:VAL:HG11  | 1.60                     | 0.83              |
| 40:J:59:LYS:HE2   | 40:J:62:ARG:HH21   | 1.44                     | 0.83              |
| 7:10:3:LEU:HD12   | 7:10:6:GLN:H       | 1.41                     | 0.83              |
| 20:23:82:VAL:HG12 | 20:23:83:GLY:H     | 1.40                     | 0.83              |
| 44:N:92:ILE:H     | 44:N:92:ILE:HD12   | 1.42                     | 0.83              |
| 51:U:49:ALA:O     | 51:U:52:VAL:HG12   | 1.77                     | 0.83              |
| 42:L:39:THR:HG22  | 42:L:40:THR:H      | 1.42                     | 0.83              |
| 54:01:1300:G:H4'  | 54:01:1301:A:H5'   | 1.61                     | 0.83              |
| 34:D:131:ILE:H    | 34:D:131:ILE:HD12  | 1.44                     | 0.83              |
| 46:P:28:ARG:HE    | 46:P:29:ASN:HD21   | 1.25                     | 0.83              |
| 11:14:101:ILE:HB  | 11:14:105:ILE:HG13 | 1.61                     | 0.82              |
| 41:K:121:ARG:NH2  | 51:U:35:GLU:HG2    | 1.94                     | 0.82              |
| 2:05:34:VAL:HA    | 2:05:50:VAL:HG12   | 1.62                     | 0.82              |
| 9:12:59:ALA:O     | 9:12:62:VAL:HG12   | 1.79                     | 0.82              |
| 33:C:39:ARG:NH1   | 33:C:54:ILE:HG13   | 1.95                     | 0.82              |
| 36:F:66:ALA:HB1   | 36:F:67:PRO:HD2    | 1.62                     | 0.82              |
| 40:J:10:LEU:HD11  | 40:J:72:ARG:HB2    | 1.62                     | 0.82              |
| 6:09:63:ALA:HA    | 6:09:66:ASN:HD22   | 1.43                     | 0.81              |
| 53:A:1033:G:H2'   | 53:A:1034:G:H5''   | 1.62                     | 0.81              |
| 54:01:215:G:H4'   | 54:01:216:A:H4'    | 1.61                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:18:3:ILE:H     | 15:18:3:ILE:HD12  | 1.44                     | 0.81              |
| 33:C:112:ALA:HB2  | 33:C:182:ASP:HB3  | 1.60                     | 0.81              |
| 33:C:6:PRO:HG2    | 33:C:200:TRP:HE1  | 1.43                     | 0.81              |
| 34:D:36:ALA:H     | 34:D:37:PRO:HD3   | 1.45                     | 0.81              |
| 33:C:96:VAL:HB    | 33:C:97:PRO:HD2   | 1.61                     | 0.81              |
| 3:06:24:ASN:HD22  | 3:06:27:LEU:HB2   | 1.46                     | 0.80              |
| 16:19:49:ARG:NH2  | 17:20:72:VAL:HG13 | 1.96                     | 0.80              |
| 2:05:121:THR:HG21 | 2:05:143:PRO:HB3  | 1.64                     | 0.80              |
| 12:15:12:MET:HA   | 54:01:910:A:H62   | 1.46                     | 0.80              |
| 6:09:79:THR:HG23  | 6:09:147:VAL:HG21 | 1.64                     | 0.80              |
| 31:34:23:ILE:HD13 | 54:01:1032:A:H1'  | 1.63                     | 0.80              |
| 34:D:187:ARG:HH22 | 34:D:192:ALA:HA   | 1.44                     | 0.80              |
| 54:01:1133:A:H4'  | 54:01:1134:A:H5'' | 1.63                     | 0.80              |
| 2:05:110:THR:HB   | 2:05:202:ILE:HB   | 1.62                     | 0.80              |
| 38:H:77:VAL:HG12  | 38:H:84:ILE:HD12  | 1.64                     | 0.80              |
| 30:33:41:ARG:HA   | 30:33:44:ARG:HH12 | 1.46                     | 0.80              |
| 54:01:807:U:H2'   | 54:01:808:G:H8    | 1.44                     | 0.80              |
| 4:07:107:VAL:HB   | 4:07:108:PRO:HD3  | 1.63                     | 0.80              |
| 32:B:15:PHE:HB3   | 59:Z:43:LYS:HB2   | 1.63                     | 0.80              |
| 10:13:102:PRO:HB3 | 10:13:121:GLU:HB3 | 1.63                     | 0.79              |
| 20:23:73:ASN:ND2  | 20:23:76:THR:H    | 1.79                     | 0.79              |
| 1:04:234:GLY:HA2  | 1:04:238:ASN:HD22 | 1.44                     | 0.79              |
| 4:07:52:ALA:HA    | 4:07:55:ASP:OD2   | 1.81                     | 0.79              |
| 43:M:6:ILE:HG13   | 43:M:7:ASN:H      | 1.47                     | 0.79              |
| 52:03:4:LEU:HD12  | 52:03:12:ARG:HD2  | 1.63                     | 0.79              |
| 53:A:211:G:H2'    | 53:A:212:G:H5'    | 1.63                     | 0.79              |
| 19:22:40:LYS:HD2  | 54:01:1598:A:H5'' | 1.64                     | 0.79              |
| 46:P:19:VAL:HG13  | 46:P:36:VAL:O     | 1.82                     | 0.79              |
| 11:14:63:LYS:HA   | 30:33:12:ARG:HG2  | 1.65                     | 0.79              |
| 19:22:39:THR:OG1  | 19:22:42:GLU:HG3  | 1.82                     | 0.79              |
| 35:E:54:GLU:HG2   | 35:E:56:PRO:HD2   | 1.64                     | 0.79              |
| 40:J:20:GLN:O     | 40:J:24:GLU:HG3   | 1.83                     | 0.79              |
| 4:07:64:PRO:HA    | 4:07:88:VAL:HG22  | 1.62                     | 0.79              |
| 53:A:1201:A:H1'   | 53:A:1202:U:OP2   | 1.81                     | 0.79              |
| 53:A:112:G:H21    | 53:A:354:G:H5'    | 1.47                     | 0.78              |
| 47:Q:13:SER:H     | 47:Q:21:VAL:HG13  | 1.46                     | 0.78              |
| 54:01:742:A:H2'   | 54:01:743:A:H8    | 1.47                     | 0.78              |
| 52:03:64:VAL:HG22 | 52:03:160:GLN:HG3 | 1.65                     | 0.78              |
| 3:06:112:LEU:HB3  | 3:06:118:LEU:HB2  | 1.64                     | 0.78              |
| 32:B:205:ALA:HA   | 59:Z:45:GLU:OE2   | 1.83                     | 0.78              |
| 33:C:9:ILE:HD13   | 44:N:97:LYS:HD3   | 1.64                     | 0.78              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:M:3:ILE:HD11   | 43:M:21:ILE:HD11   | 1.66                     | 0.78              |
| 5:08:34:ARG:HE    | 5:08:70:LEU:HD13   | 1.48                     | 0.78              |
| 13:16:100:CYS:HA  | 27:30:42:ILE:HG12  | 1.66                     | 0.78              |
| 14:17:17:LYS:NZ   | 54:01:2380:C:H5'   | 1.98                     | 0.78              |
| 44:N:25:GLU:HB2   | 44:N:29:ILE:HD12   | 1.66                     | 0.78              |
| 33:C:131:ARG:HE   | 33:C:135:ARG:HH21  | 1.29                     | 0.78              |
| 35:E:133:ILE:O    | 35:E:136:VAL:HG12  | 1.84                     | 0.78              |
| 42:L:86:VAL:HG23  | 42:L:88:ASP:H      | 1.49                     | 0.78              |
| 55:02:3:C:C2'     | 55:02:4:C:H5''     | 2.13                     | 0.78              |
| 32:B:165:ALA:HB3  | 32:B:190:SER:HB3   | 1.65                     | 0.78              |
| 9:12:78:THR:HG22  | 54:01:2641:G:H5''  | 1.66                     | 0.78              |
| 18:21:82:MET:HB3  | 18:21:84:ARG:HH22  | 1.49                     | 0.78              |
| 2:05:49:GLN:HE21  | 2:05:79:LEU:HD13   | 1.49                     | 0.77              |
| 11:14:95:LEU:HD22 | 11:14:100:ILE:HD11 | 1.66                     | 0.77              |
| 33:C:150:VAL:HG12 | 33:C:199:VAL:HG23  | 1.65                     | 0.77              |
| 40:J:65:TYR:HB3   | 44:N:95:LEU:HD11   | 1.66                     | 0.77              |
| 54:01:1668:A:H61  | 54:01:1676:A:H61   | 1.30                     | 0.77              |
| 53:A:1513:A:H2'   | 53:A:1514:G:H8     | 1.48                     | 0.77              |
| 16:19:8:ILE:HD12  | 16:19:9:ALA:N      | 2.00                     | 0.77              |
| 44:N:7:ALA:O      | 44:N:10:VAL:HG12   | 1.84                     | 0.77              |
| 46:P:28:ARG:HE    | 46:P:29:ASN:ND2    | 1.82                     | 0.77              |
| 1:04:116:GLN:HE21 | 1:04:121:ALA:HA    | 1.49                     | 0.77              |
| 4:07:92:GLY:O     | 4:07:95:MET:HG2    | 1.85                     | 0.77              |
| 20:23:65:GLN:HE21 | 54:01:328:U:H4'    | 1.50                     | 0.77              |
| 38:H:29:SER:HB3   | 38:H:32:LYS:HG2    | 1.67                     | 0.77              |
| 6:09:87:GLU:HG2   | 36:F:21:MET:HE3    | 1.67                     | 0.77              |
| 31:34:26:ILE:HD12 | 31:34:26:ILE:O     | 1.84                     | 0.77              |
| 1:04:86:ARG:HH12  | 54:01:1817:G:H5''  | 1.49                     | 0.77              |
| 12:15:42:THR:OG1  | 12:15:45:GLN:HG3   | 1.85                     | 0.77              |
| 43:M:27:THR:HA    | 43:M:30:LYS:HE2    | 1.65                     | 0.77              |
| 52:03:10:VAL:HG12 | 52:03:14:LYS:HE3   | 1.66                     | 0.77              |
| 54:01:1053:C:H2'  | 54:01:1054:A:H5''  | 1.67                     | 0.77              |
| 34:D:124:VAL:HG23 | 34:D:141:VAL:O     | 1.84                     | 0.76              |
| 37:G:6:ILE:HD12   | 37:G:6:ILE:O       | 1.85                     | 0.76              |
| 42:L:23:LEU:HB3   | 42:L:26:CYS:SG     | 2.24                     | 0.76              |
| 54:01:805:G:H22   | 54:01:828:U:H5''   | 1.48                     | 0.76              |
| 1:04:260:LYS:HA   | 1:04:263:ASP:OD2   | 1.83                     | 0.76              |
| 12:15:75:GLU:HB3  | 12:15:90:GLU:HG3   | 1.67                     | 0.76              |
| 33:C:133:MET:HE3  | 33:C:167:TYR:HB2   | 1.67                     | 0.76              |
| 14:17:49:VAL:HG21 | 14:17:82:ALA:HA    | 1.65                     | 0.76              |
| 34:D:25:ARG:HH22  | 34:D:30:LYS:HZ1    | 1.33                     | 0.76              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:E:89:THR:CG2   | 35:E:134:ASN:HD21  | 1.98                     | 0.76              |
| 54:01:1141:U:H4'  | 54:01:1142:A:O4'   | 1.84                     | 0.76              |
| 37:G:111:GLY:HA2  | 37:G:118:ARG:HD3   | 1.68                     | 0.76              |
| 48:R:29:LYS:NZ    | 59:Z:145:LEU:HD21  | 1.99                     | 0.76              |
| 35:E:148:SER:HB2  | 35:E:149:PRO:HD2   | 1.65                     | 0.76              |
| 47:Q:45:VAL:HG21  | 47:Q:60:ILE:HD13   | 1.64                     | 0.76              |
| 53:A:950:U:H2'    | 53:A:951:G:H8      | 1.50                     | 0.76              |
| 40:J:100:ILE:HD12 | 40:J:100:ILE:O     | 1.86                     | 0.76              |
| 41:K:87:GLY:H     | 41:K:113:THR:HG22  | 1.49                     | 0.76              |
| 51:U:58:LYS:HG3   | 51:U:61:ARG:HE     | 1.51                     | 0.76              |
| 9:12:31:GLU:HG2   | 9:12:142:ILE:HG12  | 1.65                     | 0.76              |
| 9:12:64:VAL:HB    | 9:12:68:LYS:HE3    | 1.66                     | 0.76              |
| 54:01:2296:U:H5'' | 54:01:2297:A:OP1   | 1.86                     | 0.76              |
| 34:D:81:LEU:HD12  | 34:D:88:ASN:HB3    | 1.68                     | 0.76              |
| 54:01:1906:G:H2'  | 54:01:1907:G:H5''  | 1.66                     | 0.76              |
| 32:B:202:ASN:HA   | 59:Z:43:LYS:HZ1    | 1.48                     | 0.76              |
| 44:N:26:LEU:HD23  | 44:N:47:LEU:HD13   | 1.68                     | 0.75              |
| 8:11:20:SER:HB3   | 8:11:21:PRO:HD3    | 1.68                     | 0.75              |
| 10:13:69:VAL:HG21 | 10:13:104:THR:HG21 | 1.67                     | 0.75              |
| 21:24:75:GLN:HB2  | 21:24:92:VAL:HG23  | 1.69                     | 0.75              |
| 25:28:4:ILE:HD11  | 25:28:56:VAL:CG2   | 2.15                     | 0.75              |
| 46:P:14:ARG:HH12  | 53:A:618:C:H1'     | 1.51                     | 0.75              |
| 52:03:52:ALA:HB1  | 52:03:167:LYS:HA   | 1.69                     | 0.75              |
| 53:A:327:A:O2'    | 53:A:328:C:H4'     | 1.87                     | 0.75              |
| 39:I:20:ILE:CD1   | 39:I:60:LEU:HD22   | 2.17                     | 0.75              |
| 41:K:92:ARG:O     | 41:K:95:THR:HG22   | 1.87                     | 0.75              |
| 4:07:28:PRO:HB2   | 4:07:168:LEU:HD13  | 1.69                     | 0.75              |
| 8:11:34:ILE:HD12  | 8:11:34:ILE:H      | 1.51                     | 0.75              |
| 8:11:100:ILE:HG22 | 8:11:101:SER:H     | 1.49                     | 0.75              |
| 9:12:47:HIS:ND1   | 9:12:48:VAL:HG23   | 2.01                     | 0.75              |
| 32:B:27:LYS:HB3   | 32:B:28:PRO:HD3    | 1.69                     | 0.75              |
| 43:M:76:ILE:HG22  | 43:M:80:MET:HE2    | 1.69                     | 0.75              |
| 7:10:47:GLU:OE2   | 7:10:95:LEU:HD11   | 1.87                     | 0.74              |
| 17:20:49:ILE:HB   | 17:20:51:VAL:O     | 1.87                     | 0.74              |
| 39:I:91:GLU:HA    | 39:I:94:ARG:HB2    | 1.68                     | 0.74              |
| 35:E:82:HIS:HD2   | 38:H:98:LEU:HD21   | 1.52                     | 0.74              |
| 44:N:37:ASP:OD1   | 44:N:39:ASP:HB3    | 1.86                     | 0.74              |
| 9:12:11:VAL:HG21  | 9:12:50:THR:HG22   | 1.69                     | 0.74              |
| 33:C:156:LEU:HD12 | 33:C:156:LEU:O     | 1.87                     | 0.74              |
| 35:E:164:LEU:HD12 | 35:E:165:GLY:N     | 2.03                     | 0.74              |
| 42:L:77:SER:HB2   | 42:L:102:ASP:HB3   | 1.70                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:03:57:GLN:HE21 | 52:03:204:ALA:HA  | 1.51                     | 0.74              |
| 27:30:51:ARG:HB2  | 27:30:51:ARG:NH2  | 2.02                     | 0.74              |
| 51:U:8:ASN:HB3    | 51:U:9:GLU:OE1    | 1.87                     | 0.74              |
| 52:03:6:LYS:HG3   | 52:03:7:ARG:H     | 1.52                     | 0.74              |
| 52:03:195:ALA:HA  | 52:03:198:LYS:HD2 | 1.68                     | 0.74              |
| 54:01:807:U:H2'   | 54:01:808:G:C8    | 2.22                     | 0.74              |
| 54:01:1645:G:H5'' | 54:01:1646:C:H5'  | 1.68                     | 0.74              |
| 56:X:13:C:C2'     | 56:X:14:A:H5''    | 2.14                     | 0.74              |
| 36:F:89:VAL:HG12  | 36:F:90:MET:H     | 1.52                     | 0.74              |
| 2:05:145:SER:HB2  | 54:01:2578:G:N7   | 2.02                     | 0.74              |
| 3:06:117:ARG:HH21 | 3:06:184:ASP:HA   | 1.52                     | 0.74              |
| 6:09:58:LEU:O     | 6:09:61:VAL:HG22  | 1.87                     | 0.74              |
| 6:09:73:ASN:HB2   | 6:09:108:VAL:HG23 | 1.69                     | 0.74              |
| 2:05:49:GLN:NE2   | 2:05:79:LEU:HD13  | 2.03                     | 0.74              |
| 54:01:2553:G:H3'  | 54:01:2554:U:H5'' | 1.69                     | 0.74              |
| 32:B:134:LEU:HG   | 32:B:138:ARG:HE   | 1.52                     | 0.74              |
| 51:U:65:ARG:HB2   | 51:U:67:THR:HG22  | 1.69                     | 0.74              |
| 54:01:742:A:H2'   | 54:01:743:A:C8    | 2.21                     | 0.74              |
| 3:06:149:ILE:HG21 | 3:06:188:MET:HG2  | 1.70                     | 0.73              |
| 5:08:102:ILE:HB   | 5:08:114:HIS:HB3  | 1.71                     | 0.73              |
| 16:19:108:LEU:HA  | 17:20:48:LYS:NZ   | 2.02                     | 0.73              |
| 45:O:24:THR:HG21  | 45:O:69:LEU:HD13  | 1.69                     | 0.73              |
| 48:R:29:LYS:HZ1   | 59:Z:145:LEU:HD21 | 1.52                     | 0.73              |
| 53:A:1418:A:H3'   | 53:A:1419:G:H5''  | 1.68                     | 0.73              |
| 9:12:80:HIS:ND1   | 9:12:81:ILE:HG22  | 2.02                     | 0.73              |
| 54:01:2277:G:C2'  | 54:01:2278:A:H5'' | 2.18                     | 0.73              |
| 54:01:2452:C:H42  | 54:01:2504:U:H3   | 1.33                     | 0.73              |
| 1:04:77:VAL:HG21  | 1:04:109:LEU:HD11 | 1.70                     | 0.73              |
| 53:A:405:U:H3'    | 53:A:406:G:H5'    | 1.70                     | 0.73              |
| 43:M:113:LYS:N    | 43:M:114:PRO:HD2  | 2.04                     | 0.73              |
| 13:16:79:LEU:HD23 | 13:16:83:LEU:HD12 | 1.70                     | 0.73              |
| 47:Q:16:MET:HG3   | 47:Q:19:SER:OG    | 1.88                     | 0.73              |
| 2:05:81:GLU:HG2   | 2:05:82:PHE:H     | 1.53                     | 0.73              |
| 4:07:90:LEU:HD12  | 4:07:90:LEU:O     | 1.89                     | 0.73              |
| 12:15:45:GLN:NE2  | 54:01:2485:G:H5'' | 2.03                     | 0.73              |
| 14:17:17:LYS:HZ1  | 54:01:2380:C:H5'  | 1.51                     | 0.73              |
| 14:17:105:ALA:HA  | 14:17:108:ASP:OD2 | 1.89                     | 0.73              |
| 16:19:108:LEU:HA  | 17:20:48:LYS:HZ3  | 1.52                     | 0.73              |
| 33:C:10:ARG:HG2   | 33:C:177:LEU:HD23 | 1.69                     | 0.73              |
| 34:D:70:GLN:HA    | 34:D:73:ASN:HD22  | 1.54                     | 0.73              |
| 36:F:48:ALA:HB1   | 48:R:68:PRO:HG3   | 1.71                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:11:93:ASN:ND2    | 54:01:1077:A:H4'   | 2.04                     | 0.73              |
| 33:C:122:GLN:HB3   | 33:C:127:VAL:HG11  | 1.71                     | 0.73              |
| 10:13:21:CYS:HA    | 10:13:41:ILE:HG22  | 1.70                     | 0.72              |
| 36:F:38:ARG:HB3    | 36:F:40:GLU:OE2    | 1.89                     | 0.72              |
| 45:O:17:ASP:OD1    | 45:O:20:ASP:HB2    | 1.89                     | 0.72              |
| 1:04:154:ALA:HA    | 1:04:159:THR:HG21  | 1.69                     | 0.72              |
| 34:D:8:LEU:HD23    | 53:A:429:U:H5'     | 1.70                     | 0.72              |
| 39:I:45:MET:HB3    | 39:I:48:ARG:HH21   | 1.52                     | 0.72              |
| 42:L:31:GLY:O      | 42:L:78:VAL:HG13   | 1.89                     | 0.72              |
| 4:07:137:PHE:HB2   | 4:07:140:ILE:HD13  | 1.71                     | 0.72              |
| 8:11:21:PRO:HB2    | 8:11:22:PRO:HD3    | 1.71                     | 0.72              |
| 10:13:76:VAL:HG12  | 15:18:72:VAL:CG2   | 2.19                     | 0.72              |
| 12:15:69:PRO:HA    | 12:15:94:ALA:HB2   | 1.68                     | 0.72              |
| 20:23:73:ASN:ND2   | 20:23:75:ALA:HB3   | 2.05                     | 0.72              |
| 53:A:279:A:H5'     | 53:A:281:G:H5'     | 1.70                     | 0.72              |
| 1:04:120:ASP:HA    | 6:09:91:PHE:HZ     | 1.53                     | 0.72              |
| 1:04:266:ILE:HG21  | 1:04:269:ARG:HD2   | 1.71                     | 0.72              |
| 50:T:11:ILE:O      | 50:T:14:GLU:HB2    | 1.89                     | 0.72              |
| 9:12:58:ASN:HD21   | 9:12:128:ASN:HB2   | 1.54                     | 0.72              |
| 27:30:24:VAL:HG13  | 27:30:25:THR:H     | 1.54                     | 0.72              |
| 35:E:76:ASN:HB2    | 35:E:81:GLN:HE22   | 1.53                     | 0.72              |
| 54:01:1906:G:C3'   | 54:01:1907:G:H5''  | 2.19                     | 0.72              |
| 59:Z:110:GLY:HA3   | 59:Z:124:LEU:HD23  | 1.70                     | 0.72              |
| 22:25:36:GLN:HE22  | 22:25:39:THR:HA    | 1.53                     | 0.72              |
| 31:34:2:LYS:HB2    | 31:34:35:GLN:HB3   | 1.71                     | 0.72              |
| 54:01:1807:G:H2'   | 54:01:1808:A:H5'   | 1.71                     | 0.72              |
| 5:08:96:ALA:HB3    | 5:08:103:ASN:HB3   | 1.70                     | 0.72              |
| 11:14:111:ILE:HD12 | 11:14:111:ILE:N    | 2.05                     | 0.72              |
| 49:S:32:THR:HG22   | 49:S:49:ALA:O      | 1.90                     | 0.72              |
| 28:31:4:ILE:H      | 28:31:4:ILE:HD12   | 1.54                     | 0.72              |
| 34:D:66:VAL:HG12   | 34:D:67:LEU:H      | 1.53                     | 0.72              |
| 51:U:64:ALA:C      | 51:U:66:ARG:H      | 1.96                     | 0.72              |
| 54:01:1060:U:H5'   | 54:01:1062:G:H5'   | 1.72                     | 0.72              |
| 34:D:12:ARG:HG2    | 34:D:33:ILE:HD12   | 1.71                     | 0.71              |
| 34:D:33:ILE:HG13   | 34:D:34:GLU:N      | 2.02                     | 0.71              |
| 9:12:98:GLU:O      | 9:12:102:GLU:HG3   | 1.89                     | 0.71              |
| 34:D:87:GLU:HG3    | 34:D:187:ARG:HD3   | 1.72                     | 0.71              |
| 15:18:88:ARG:HE    | 15:18:112:ARG:HH21 | 1.35                     | 0.71              |
| 42:L:22:ALA:HB2    | 42:L:94:TYR:CE1    | 2.26                     | 0.71              |
| 1:04:86:ARG:NH1    | 54:01:1817:G:H5''  | 2.05                     | 0.71              |
| 11:14:33:ARG:HD2   | 11:14:40:SER:HA    | 1.73                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:E:89:THR:HG21  | 35:E:134:ASN:HD21 | 1.55                     | 0.71              |
| 44:N:40:ARG:HH22  | 49:S:6:LYS:HD2    | 1.54                     | 0.71              |
| 5:08:138:GLN:HE22 | 54:01:2759:G:H21  | 1.39                     | 0.71              |
| 42:L:71:HIS:HB2   | 42:L:73:LEU:HD13  | 1.72                     | 0.71              |
| 8:11:4:VAL:HG22   | 8:11:7:TYR:HE2    | 1.56                     | 0.71              |
| 8:11:85:ILE:HD12  | 8:11:85:ILE:O     | 1.91                     | 0.71              |
| 19:22:29:THR:HG23 | 19:22:85:VAL:O    | 1.89                     | 0.71              |
| 32:B:72:LYS:NZ    | 32:B:204:ASP:HA   | 2.06                     | 0.71              |
| 31:34:2:LYS:HD2   | 31:34:4:ARG:HH12  | 1.55                     | 0.71              |
| 32:B:72:LYS:HE2   | 32:B:74:ALA:HB3   | 1.71                     | 0.71              |
| 3:06:149:ILE:HD11 | 3:06:172:ALA:HA   | 1.73                     | 0.71              |
| 11:14:32:GLY:HA2  | 54:01:1190:G:H5'' | 1.73                     | 0.71              |
| 26:29:65:ASN:O    | 26:29:66:ILE:HB   | 1.89                     | 0.71              |
| 35:E:40:ASP:OD2   | 35:E:42:ASN:HB3   | 1.90                     | 0.71              |
| 42:L:31:GLY:HA3   | 42:L:54:VAL:CG1   | 2.20                     | 0.71              |
| 24:27:2:LYS:HE2   | 54:01:102:U:H1'   | 1.73                     | 0.71              |
| 53:A:29:U:O2'     | 53:A:30:U:H5'     | 1.91                     | 0.71              |
| 54:01:2584:U:H2'  | 54:01:2585:U:H2'  | 1.73                     | 0.71              |
| 26:29:58:ASP:HA   | 26:29:61:ASN:ND2  | 2.06                     | 0.70              |
| 35:E:59:ILE:HD12  | 35:E:60:GLN:N     | 2.04                     | 0.70              |
| 7:10:13:ALA:O     | 7:10:17:GLU:HG3   | 1.91                     | 0.70              |
| 13:16:20:MET:HE1  | 13:16:40:LYS:HD3  | 1.73                     | 0.70              |
| 25:28:4:ILE:HG22  | 25:28:37:ARG:O    | 1.91                     | 0.70              |
| 41:K:15:VAL:HG12  | 41:K:76:TYR:HB3   | 1.74                     | 0.70              |
| 43:M:97:ARG:HB2   | 43:M:99:GLN:NE2   | 2.04                     | 0.70              |
| 1:04:209:ALA:HA   | 1:04:212:TRP:CE2  | 2.27                     | 0.70              |
| 3:06:46:GLN:HB3   | 3:06:83:VAL:HG21  | 1.72                     | 0.70              |
| 54:01:2286:G:H5'' | 54:01:2287:A:OP1  | 1.92                     | 0.70              |
| 2:05:3:GLY:C      | 2:05:4:LEU:HD12   | 2.16                     | 0.70              |
| 26:29:56:ARG:HH22 | 49:S:68:HIS:HE1   | 1.38                     | 0.70              |
| 34:D:23:GLY:HA2   | 34:D:108:ALA:HB1  | 1.74                     | 0.70              |
| 20:23:4:ILE:HD12  | 20:23:4:ILE:N     | 2.07                     | 0.70              |
| 49:S:30:LEU:HB2   | 49:S:48:ILE:HG22  | 1.73                     | 0.70              |
| 53:A:70:U:H5''    | 53:A:71:A:OP1     | 1.91                     | 0.70              |
| 36:F:5:GLU:HG2    | 36:F:61:LEU:HD11  | 1.74                     | 0.70              |
| 13:16:38:LEU:HD11 | 13:16:42:LYS:HE2  | 1.74                     | 0.70              |
| 34:D:36:ALA:N     | 34:D:37:PRO:HD3   | 2.06                     | 0.70              |
| 51:U:36:PHE:HB3   | 51:U:40:PRO:HD3   | 1.72                     | 0.70              |
| 8:11:76:ALA:O     | 8:11:80:LYS:HG3   | 1.92                     | 0.70              |
| 16:19:88:GLU:OE1  | 17:20:52:PRO:HD3  | 1.92                     | 0.70              |
| 55:02:65:U:H3'    | 55:02:108:A:H61   | 1.57                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:G:72:VAL:HG12   | 37:G:89:GLU:HA     | 1.72                     | 0.70              |
| 21:24:76:ASP:H     | 21:24:90:ASP:HB2   | 1.55                     | 0.69              |
| 43:M:15:VAL:HG23   | 43:M:16:ILE:H      | 1.57                     | 0.69              |
| 51:U:25:ALA:HA     | 51:U:28:LEU:HB3    | 1.73                     | 0.69              |
| 19:22:61:LEU:C     | 19:22:61:LEU:HD12  | 2.17                     | 0.69              |
| 53:A:946:A:H2'     | 53:A:947:G:H8      | 1.57                     | 0.69              |
| 54:01:679:C:H2'    | 54:01:680:C:C6     | 2.26                     | 0.69              |
| 54:01:947:A:H2'    | 54:01:948:C:C6     | 2.27                     | 0.69              |
| 54:01:971:G:H2'    | 54:01:972:A:O4'    | 1.92                     | 0.69              |
| 54:01:1906:G:C2'   | 54:01:1907:G:H5''  | 2.22                     | 0.69              |
| 52:03:16:ASP:OD2   | 52:03:19:LYS:HB2   | 1.92                     | 0.69              |
| 11:14:111:ILE:HG22 | 11:14:112:LEU:H    | 1.58                     | 0.69              |
| 14:17:89:ASP:HA    | 14:17:116:GLN:HB2  | 1.74                     | 0.69              |
| 17:20:28:ALA:HB3   | 17:20:31:GLU:HB2   | 1.75                     | 0.69              |
| 33:C:58:ARG:HG3    | 33:C:62:SER:O      | 1.92                     | 0.69              |
| 40:J:44:THR:HG23   | 40:J:69:THR:O      | 1.93                     | 0.69              |
| 43:M:3:ILE:HG12    | 43:M:7:ASN:HD22    | 1.56                     | 0.69              |
| 43:M:97:ARG:CB     | 43:M:99:GLN:HE22   | 2.02                     | 0.69              |
| 53:A:1513:A:H2'    | 53:A:1514:G:C8     | 2.26                     | 0.69              |
| 38:H:10:LEU:HD22   | 38:H:74:ILE:HD11   | 1.75                     | 0.69              |
| 38:H:36:ALA:HA     | 38:H:39:LEU:HD12   | 1.73                     | 0.69              |
| 53:A:225:C:H2'     | 53:A:226:G:H5''    | 1.75                     | 0.69              |
| 54:01:615:U:H5''   | 54:01:616:A:OP2    | 1.92                     | 0.69              |
| 25:28:29:ARG:NE    | 54:01:1183:U:H5''  | 2.07                     | 0.69              |
| 43:M:52:ILE:HG22   | 43:M:56:ARG:NH1    | 2.07                     | 0.69              |
| 1:04:153:LEU:HD13  | 1:04:175:LEU:HD21  | 1.73                     | 0.69              |
| 1:04:156:SER:OG    | 54:01:1818:U:H5'   | 1.92                     | 0.69              |
| 10:13:76:VAL:HG12  | 15:18:72:VAL:HG21  | 1.73                     | 0.69              |
| 24:27:21:LEU:HD23  | 24:27:25:GLN:HG2   | 1.74                     | 0.69              |
| 52:03:46:VAL:HG22  | 52:03:212:VAL:HA   | 1.73                     | 0.69              |
| 53:A:335:C:H2'     | 53:A:336:A:H8      | 1.57                     | 0.69              |
| 8:11:4:VAL:HG22    | 8:11:7:TYR:CE2     | 2.28                     | 0.69              |
| 52:03:26:ALA:HB1   | 52:03:214:ILE:HD11 | 1.74                     | 0.69              |
| 54:01:310:A:C2'    | 54:01:311:A:H5''   | 2.21                     | 0.69              |
| 7:10:11:ILE:O      | 7:10:15:VAL:HG23   | 1.93                     | 0.69              |
| 39:I:24:ASN:ND2    | 39:I:26:LYS:HB3    | 2.08                     | 0.69              |
| 50:T:59:ARG:NH1    | 53:A:177:G:H5'     | 2.07                     | 0.69              |
| 45:O:21:THR:HG21   | 53:A:658:C:H1'     | 1.74                     | 0.68              |
| 53:A:1379:G:O2'    | 53:A:1380:U:H5'    | 1.94                     | 0.68              |
| 8:11:91:LYS:HG2    | 8:11:94:LYS:HE2    | 1.75                     | 0.68              |
| 28:31:46:VAL:HG12  | 28:31:47:ILE:H     | 1.57                     | 0.68              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 54:01:467:G:O2'    | 54:01:468:G:H5'   | 1.94                     | 0.68              |
| 54:01:2086:U:H2'   | 54:01:2087:G:C8   | 2.28                     | 0.68              |
| 1:04:229:HIS:HE2   | 1:04:246:PRO:HG3  | 1.58                     | 0.68              |
| 7:10:34:THR:O      | 7:10:37:LYS:HG2   | 1.93                     | 0.68              |
| 29:32:26:ASN:O     | 29:32:30:VAL:HG23 | 1.92                     | 0.68              |
| 3:06:148:ILE:HB    | 3:06:169:VAL:HG22 | 1.74                     | 0.68              |
| 7:10:97:LYS:HZ1    | 7:10:129:LEU:HB2  | 1.58                     | 0.68              |
| 18:21:11:ARG:HD3   | 54:01:1322:A:OP1  | 1.94                     | 0.68              |
| 39:I:20:ILE:HD11   | 39:I:60:LEU:CD2   | 2.20                     | 0.68              |
| 41:K:15:VAL:HG22   | 41:K:16:SER:H     | 1.59                     | 0.68              |
| 46:P:10:GLY:HA2    | 53:A:624:C:H4'    | 1.74                     | 0.68              |
| 53:A:950:U:H2'     | 53:A:951:G:C8     | 2.28                     | 0.68              |
| 54:01:704:G:H2'    | 54:01:726:G:N2    | 2.09                     | 0.68              |
| 53:A:1506:U:O2'    | 53:A:1507:A:H5'   | 1.93                     | 0.68              |
| 32:B:182:VAL:HB    | 32:B:195:VAL:HG13 | 1.75                     | 0.68              |
| 35:E:23:THR:HA     | 35:E:28:ARG:HA    | 1.76                     | 0.68              |
| 42:L:109:ARG:NH1   | 53:A:537:G:H5''   | 2.08                     | 0.68              |
| 43:M:16:ILE:HD12   | 43:M:16:ILE:H     | 1.57                     | 0.68              |
| 1:04:149:LYS:HD3   | 54:01:2204:G:H4'  | 1.75                     | 0.68              |
| 1:04:206:LYS:HD2   | 54:01:729:G:OP2   | 1.94                     | 0.68              |
| 1:04:259:ASN:OD1   | 1:04:261:ARG:HG2  | 1.93                     | 0.68              |
| 9:12:81:ILE:HG13   | 9:12:82:GLY:N     | 2.09                     | 0.68              |
| 51:U:24:LYS:HG2    | 51:U:25:ALA:N     | 2.09                     | 0.68              |
| 35:E:113:VAL:HG13  | 35:E:114:LEU:HD12 | 1.75                     | 0.68              |
| 46:P:51:ARG:C      | 46:P:52:LEU:HD12  | 2.18                     | 0.68              |
| 53:A:1218:C:H2'    | 53:A:1219:A:C8    | 2.28                     | 0.68              |
| 54:01:1373:A:H5'   | 54:01:2212:A:H1'  | 1.76                     | 0.68              |
| 3:06:149:ILE:HG23  | 3:06:188:MET:HA   | 1.76                     | 0.67              |
| 27:30:51:ARG:HG2   | 27:30:53:VAL:HG13 | 1.74                     | 0.67              |
| 3:06:105:LEU:HD23  | 3:06:108:ILE:HD12 | 1.76                     | 0.67              |
| 7:10:116:GLU:O     | 7:10:119:PRO:HD2  | 1.94                     | 0.67              |
| 27:30:24:VAL:HG22  | 27:30:26:SER:H    | 1.58                     | 0.67              |
| 14:17:10:ARG:HD3   | 54:01:2295:C:OP2  | 1.95                     | 0.67              |
| 43:M:65:GLU:HG3    | 43:M:66:GLY:H     | 1.59                     | 0.67              |
| 46:P:28:ARG:NE     | 46:P:29:ASN:HD21  | 1.91                     | 0.67              |
| 49:S:18:VAL:O      | 49:S:22:VAL:HG23  | 1.95                     | 0.67              |
| 51:U:64:ALA:C      | 51:U:66:ARG:N     | 2.50                     | 0.67              |
| 54:01:329:G:O4'    | 54:01:477:A:H1'   | 1.93                     | 0.67              |
| 3:06:109:LEU:HG    | 3:06:112:LEU:HD12 | 1.75                     | 0.67              |
| 11:14:111:ILE:HG22 | 11:14:112:LEU:N   | 2.09                     | 0.67              |
| 20:23:96:LYS:C     | 20:23:98:ASN:H    | 2.02                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:03:7:ARG:NH2   | 52:03:11:ILE:HD11 | 2.10                     | 0.67              |
| 2:05:5:VAL:H      | 2:05:32:ASN:HD21  | 1.43                     | 0.67              |
| 8:11:7:TYR:HB3    | 8:11:59:THR:HA    | 1.77                     | 0.67              |
| 20:23:73:ASN:HD21 | 20:23:75:ALA:HB3  | 1.59                     | 0.67              |
| 35:E:96:GLN:HG2   | 35:E:97:PRO:HD2   | 1.77                     | 0.67              |
| 38:H:98:LEU:HD12  | 38:H:99:GLY:N     | 2.10                     | 0.67              |
| 59:Z:120:PHE:CE2  | 59:Z:136:VAL:HG11 | 2.29                     | 0.67              |
| 2:05:123:LYS:HE2  | 13:16:1:MET:HE1   | 1.76                     | 0.67              |
| 32:B:6:ARG:HH12   | 59:Z:8:LEU:HD22   | 1.58                     | 0.67              |
| 11:14:23:ILE:HD12 | 11:14:23:ILE:N    | 2.10                     | 0.67              |
| 15:18:95:LYS:HZ3  | 54:01:2847:U:P    | 2.16                     | 0.67              |
| 59:Z:7:GLN:O      | 59:Z:11:GLU:HG3   | 1.94                     | 0.67              |
| 41:K:126:ARG:HH22 | 53:A:692:U:H5''   | 1.59                     | 0.67              |
| 10:13:41:ILE:C    | 10:13:41:ILE:HD12 | 2.20                     | 0.67              |
| 13:16:38:LEU:HB3  | 13:16:39:PRO:HD3  | 1.76                     | 0.67              |
| 15:18:32:VAL:HG12 | 15:18:34:GLY:H    | 1.59                     | 0.67              |
| 33:C:67:ILE:HB    | 33:C:102:ILE:HG22 | 1.76                     | 0.67              |
| 54:01:466:A:H2'   | 54:01:467:G:H5'   | 1.77                     | 0.67              |
| 23:26:56:ARG:O    | 23:26:59:ASP:HB3  | 1.95                     | 0.67              |
| 35:E:133:ILE:H    | 35:E:133:ILE:CD1  | 2.06                     | 0.67              |
| 53:A:50:A:H4'     | 53:A:51:A:H5'     | 1.76                     | 0.67              |
| 53:A:411:A:C4     | 53:A:413:G:H1'    | 2.30                     | 0.67              |
| 1:04:153:LEU:HD11 | 1:04:181:ARG:NH2  | 2.11                     | 0.66              |
| 3:06:117:ARG:HH12 | 11:14:2:ARG:HB2   | 1.61                     | 0.66              |
| 9:12:101:ILE:H    | 9:12:101:ILE:HD12 | 1.60                     | 0.66              |
| 13:16:47:VAL:O    | 13:16:50:PRO:HD2  | 1.94                     | 0.66              |
| 30:33:41:ARG:HA   | 30:33:44:ARG:NH1  | 2.10                     | 0.66              |
| 54:01:1571:A:H2'  | 54:01:1572:A:C8   | 2.31                     | 0.66              |
| 19:22:28:ASN:OD1  | 19:22:91:GLN:HG3  | 1.95                     | 0.66              |
| 52:03:15:VAL:HG23 | 52:03:33:LEU:HD21 | 1.77                     | 0.66              |
| 54:01:1105:U:H2'  | 54:01:1106:G:H5'' | 1.78                     | 0.66              |
| 1:04:71:ASP:O     | 1:04:73:ILE:HG13  | 1.94                     | 0.66              |
| 37:G:75:LYS:HD3   | 37:G:88:VAL:HG11  | 1.76                     | 0.66              |
| 43:M:25:GLY:H     | 53:A:1329:A:H5''  | 1.61                     | 0.66              |
| 47:Q:6:THR:C      | 47:Q:7:LEU:HD12   | 2.20                     | 0.66              |
| 33:C:110:LEU:HD21 | 33:C:144:GLY:O    | 1.95                     | 0.66              |
| 53:A:1287:A:H2    | 53:A:1353:G:H1'   | 1.60                     | 0.66              |
| 54:01:704:G:H2'   | 54:01:726:G:H22   | 1.60                     | 0.66              |
| 7:10:37:LYS:O     | 7:10:41:LEU:HB2   | 1.95                     | 0.66              |
| 31:34:13:ASN:OD1  | 31:34:29:ALA:HB2  | 1.96                     | 0.66              |
| 38:H:95:MET:C     | 38:H:97:GLY:H     | 2.04                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:A:1391:U:H2'    | 53:A:1392:G:H8     | 1.61                     | 0.66              |
| 54:01:974:G:H1'    | 54:01:975:A:C8     | 2.31                     | 0.66              |
| 54:01:1153:C:H2'   | 54:01:1154:G:O4'   | 1.96                     | 0.66              |
| 54:01:1539:U:H2'   | 54:01:1540:G:H8    | 1.58                     | 0.66              |
| 11:14:76:GLU:C     | 11:14:77:ILE:HD12  | 2.21                     | 0.66              |
| 54:01:310:A:H2'    | 54:01:311:A:H5''   | 1.76                     | 0.66              |
| 54:01:774:G:C2'    | 54:01:775:G:H5''   | 2.26                     | 0.66              |
| 7:10:27:VAL:O      | 7:10:83:ALA:HB3    | 1.96                     | 0.66              |
| 22:25:19:VAL:HG22  | 22:25:34:VAL:HG22  | 1.78                     | 0.66              |
| 35:E:10:LEU:HD12   | 35:E:11:GLN:N      | 2.11                     | 0.66              |
| 51:U:48:LYS:HA     | 51:U:51:ALA:HB3    | 1.77                     | 0.66              |
| 18:21:31:GLN:O     | 18:21:35:ILE:HG13  | 1.95                     | 0.66              |
| 23:26:31:ASN:HD22  | 23:26:52:ALA:HB2   | 1.59                     | 0.66              |
| 38:H:29:SER:HB3    | 38:H:32:LYS:CG     | 2.26                     | 0.66              |
| 46:P:18:GLN:NE2    | 46:P:35:ARG:HH21   | 1.92                     | 0.66              |
| 54:01:435:C:H2'    | 54:01:436:C:H5'    | 1.77                     | 0.66              |
| 30:33:57:VAL:HA    | 30:33:60:CYS:SG    | 2.36                     | 0.66              |
| 31:34:1:MET:HB3    | 31:34:34:LYS:HE2   | 1.77                     | 0.66              |
| 53:A:1512:U:H2'    | 53:A:1513:A:C8     | 2.30                     | 0.66              |
| 3:06:178:VAL:HG13  | 3:06:179:SER:H     | 1.61                     | 0.66              |
| 10:13:35:VAL:HG22  | 10:13:69:VAL:HG12  | 1.78                     | 0.66              |
| 13:16:65:LEU:O     | 13:16:68:ALA:HB3   | 1.96                     | 0.66              |
| 14:17:99:TYR:HA    | 14:17:103:VAL:HG21 | 1.78                     | 0.66              |
| 21:24:42:LEU:O     | 21:24:42:LEU:HD12  | 1.97                     | 0.66              |
| 41:K:126:ARG:NH2   | 53:A:692:U:H5''    | 2.11                     | 0.66              |
| 6:09:37:VAL:O      | 6:09:39:ALA:N      | 2.28                     | 0.65              |
| 8:11:107:GLU:O     | 8:11:110:GLN:HG2   | 1.96                     | 0.65              |
| 15:18:3:ILE:HD12   | 15:18:3:ILE:N      | 2.12                     | 0.65              |
| 15:18:20:ARG:HD3   | 15:18:112:ARG:HH12 | 1.61                     | 0.65              |
| 38:H:17:GLN:HE21   | 38:H:71:VAL:HB     | 1.61                     | 0.65              |
| 40:J:86:ALA:O      | 40:J:90:LEU:HB2    | 1.96                     | 0.65              |
| 52:03:173:THR:HG21 | 52:03:192:LEU:HD21 | 1.78                     | 0.65              |
| 54:01:45:G:C5'     | 54:01:46:G:H5'     | 2.14                     | 0.65              |
| 9:12:29:ALA:HA     | 9:12:32:LEU:HD12   | 1.78                     | 0.65              |
| 17:20:74:ILE:N     | 17:20:74:ILE:HD12  | 2.12                     | 0.65              |
| 27:30:37:HIS:CD2   | 27:30:43:THR:HG22  | 2.31                     | 0.65              |
| 34:D:131:ILE:HD12  | 34:D:131:ILE:N     | 2.10                     | 0.65              |
| 48:R:25:ILE:C      | 48:R:25:ILE:HD12   | 2.20                     | 0.65              |
| 49:S:17:LYS:HG2    | 49:S:30:LEU:HD23   | 1.78                     | 0.65              |
| 2:05:81:GLU:HG2    | 2:05:82:PHE:N      | 2.11                     | 0.65              |
| 3:06:154:ASP:OD1   | 3:06:157:LEU:HB3   | 1.95                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:11:91:LYS:HB2   | 8:11:95:ASP:OD1    | 1.96                     | 0.65              |
| 17:20:39:LEU:O    | 17:20:49:ILE:HG23  | 1.97                     | 0.65              |
| 31:34:23:ILE:CD1  | 54:01:1032:A:H1'   | 2.26                     | 0.65              |
| 37:G:112:ASP:O    | 37:G:113:LYS:HD3   | 1.94                     | 0.65              |
| 54:01:796:C:H2'   | 54:01:797:G:H8     | 1.61                     | 0.65              |
| 55:02:66:A:H5''   | 55:02:67:G:OP1     | 1.95                     | 0.65              |
| 16:19:50:ARG:HH11 | 16:19:50:ARG:HG3   | 1.62                     | 0.65              |
| 53:A:245:U:O2'    | 53:A:246:A:H5'     | 1.96                     | 0.65              |
| 3:06:90:GLN:HE21  | 3:06:92:HIS:CE1    | 2.14                     | 0.65              |
| 13:16:22:ARG:HH22 | 54:01:2709:G:H5'   | 1.62                     | 0.65              |
| 13:16:90:ARG:NE   | 13:16:116:VAL:HG11 | 2.11                     | 0.65              |
| 16:19:91:ARG:HH11 | 16:19:91:ARG:HG3   | 1.62                     | 0.65              |
| 38:H:8:ASP:O      | 38:H:11:THR:HG22   | 1.97                     | 0.65              |
| 54:01:554:U:H2'   | 54:01:555:G:O4'    | 1.96                     | 0.65              |
| 18:21:42:LYS:HB2  | 54:01:2010:G:H5''  | 1.76                     | 0.65              |
| 35:E:96:GLN:CG    | 35:E:97:PRO:HD2    | 2.27                     | 0.65              |
| 46:P:5:ARG:HH11   | 53:A:376:G:H4'     | 1.62                     | 0.65              |
| 52:03:194:VAL:O   | 52:03:198:LYS:HG3  | 1.97                     | 0.65              |
| 54:01:45:G:H5''   | 54:01:46:G:C5'     | 2.15                     | 0.65              |
| 54:01:576:U:H2'   | 54:01:577:G:H8     | 1.62                     | 0.65              |
| 5:08:132:LEU:HD12 | 5:08:132:LEU:O     | 1.97                     | 0.65              |
| 48:R:41:SER:O     | 48:R:45:GLY:N      | 2.30                     | 0.65              |
| 8:11:127:SER:HA   | 54:01:1080:A:H1'   | 1.79                     | 0.65              |
| 54:01:2248:C:H2'  | 54:01:2249:U:H5'   | 1.78                     | 0.65              |
| 2:05:133:THR:O    | 2:05:134:HIS:HB2   | 1.95                     | 0.65              |
| 15:18:90:ALA:HB2  | 15:18:112:ARG:HD3  | 1.79                     | 0.65              |
| 32:B:206:ILE:HD12 | 59:Z:37:LEU:HD21   | 1.78                     | 0.65              |
| 53:A:1391:U:H2'   | 53:A:1392:G:C8     | 2.32                     | 0.65              |
| 54:01:2350:C:H2'  | 54:01:2351:G:O4'   | 1.97                     | 0.65              |
| 2:05:9:VAL:O      | 2:05:26:VAL:HB     | 1.97                     | 0.65              |
| 11:14:63:LYS:CA   | 30:33:12:ARG:HG2   | 2.26                     | 0.65              |
| 27:30:24:VAL:HG13 | 27:30:25:THR:N     | 2.12                     | 0.65              |
| 53:A:335:C:H2'    | 53:A:336:A:C8      | 2.32                     | 0.65              |
| 54:01:2800:A:H3'  | 54:01:2801:G:H5'   | 1.78                     | 0.65              |
| 39:I:117:LEU:HG   | 39:I:123:ARG:HD3   | 1.77                     | 0.64              |
| 41:K:84:MET:HG2   | 41:K:110:THR:OG1   | 1.97                     | 0.64              |
| 54:01:1053:C:C2'  | 54:01:1054:A:H5''  | 2.26                     | 0.64              |
| 1:04:62:ARG:HH11  | 1:04:62:ARG:HG3    | 1.61                     | 0.64              |
| 1:04:177:SER:HB2  | 54:01:1819:A:O2'   | 1.97                     | 0.64              |
| 7:10:67:THR:HG23  | 7:10:74:ASP:HB2    | 1.78                     | 0.64              |
| 9:12:114:LEU:O    | 9:12:117:ALA:HB3   | 1.97                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:34:37:GLN:HG3  | 31:34:38:GLY:H     | 1.62                     | 0.64              |
| 39:I:35:GLU:O     | 39:I:40:ARG:HG3    | 1.98                     | 0.64              |
| 54:01:814:C:H1'   | 54:01:1225:G:H21   | 1.61                     | 0.64              |
| 1:04:16:VAL:CB    | 1:04:203:VAL:HG22  | 2.26                     | 0.64              |
| 1:04:242:HIS:O    | 1:04:244:VAL:HG13  | 1.97                     | 0.64              |
| 21:24:9:ARG:HG2   | 21:24:41:GLU:HB2   | 1.78                     | 0.64              |
| 33:C:179:ALA:HB1  | 33:C:202:PHE:HE1   | 1.63                     | 0.64              |
| 43:M:27:THR:HG21  | 53:A:1328:C:H5''   | 1.78                     | 0.64              |
| 54:01:796:C:H2'   | 54:01:797:G:C8     | 2.32                     | 0.64              |
| 54:01:2156:G:H2'  | 54:01:2157:G:H5'   | 1.78                     | 0.64              |
| 54:01:2286:G:H4'  | 54:01:2287:A:O5'   | 1.97                     | 0.64              |
| 13:16:33:ILE:HD12 | 13:16:118:ARG:HH22 | 1.62                     | 0.64              |
| 18:21:6:LYS:HG3   | 54:01:494:G:H4'    | 1.79                     | 0.64              |
| 32:B:68:PHE:HD1   | 32:B:161:PHE:HB3   | 1.62                     | 0.64              |
| 52:03:62:ALA:HA   | 52:03:162:ARG:HA   | 1.79                     | 0.64              |
| 54:01:703:U:H2'   | 54:01:704:G:O4'    | 1.96                     | 0.64              |
| 54:01:1053:C:C3'  | 54:01:1054:A:H5''  | 2.28                     | 0.64              |
| 54:01:1571:A:H2'  | 54:01:1572:A:H8    | 1.63                     | 0.64              |
| 7:10:8:LYS:O      | 7:10:12:VAL:HG23   | 1.98                     | 0.64              |
| 33:C:59:PRO:HD2   | 33:C:62:SER:O      | 1.98                     | 0.64              |
| 54:01:197:A:H4'   | 54:01:2069:G:OP2   | 1.97                     | 0.64              |
| 54:01:1300:G:H4'  | 54:01:1301:A:C5'   | 2.26                     | 0.64              |
| 2:05:55:LYS:HD2   | 2:05:77:ARG:HA     | 1.77                     | 0.64              |
| 11:14:59:ARG:HD2  | 54:01:250:G:H4'    | 1.80                     | 0.64              |
| 14:17:52:SER:OG   | 14:17:54:VAL:HG12  | 1.96                     | 0.64              |
| 34:D:131:ILE:H    | 34:D:131:ILE:CD1   | 2.11                     | 0.64              |
| 37:G:139:ASP:O    | 37:G:143:MET:HG2   | 1.98                     | 0.64              |
| 46:P:4:ILE:HG12   | 46:P:21:VAL:HG22   | 1.79                     | 0.64              |
| 56:X:21:A:H61     | 56:X:46:G:H2'      | 1.62                     | 0.64              |
| 56:W:6:G:O2'      | 56:W:7:G:H5'       | 1.98                     | 0.64              |
| 59:Z:11:GLU:O     | 59:Z:15:GLU:HG3    | 1.98                     | 0.64              |
| 2:05:124:ARG:HA   | 2:05:165:MET:HE3   | 1.79                     | 0.64              |
| 3:06:178:VAL:HG13 | 3:06:179:SER:N     | 2.12                     | 0.64              |
| 4:07:127:TYR:HE2  | 4:07:129:MET:HE2   | 1.62                     | 0.64              |
| 8:11:100:ILE:HG22 | 8:11:101:SER:N     | 2.13                     | 0.64              |
| 8:11:123:ALA:HA   | 8:11:126:ARG:CZ    | 2.28                     | 0.64              |
| 15:18:52:ARG:HE   | 54:01:2845:U:H4'   | 1.63                     | 0.64              |
| 8:11:27:LEU:HD11  | 8:11:34:ILE:HG13   | 1.79                     | 0.64              |
| 23:26:31:ASN:ND2  | 23:26:52:ALA:HB2   | 2.13                     | 0.64              |
| 41:K:109:ILE:HG21 | 51:U:16:ARG:NH1    | 2.12                     | 0.64              |
| 46:P:12:LYS:HG2   | 46:P:13:LYS:HG2    | 1.80                     | 0.64              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:28:35:VAL:HG22  | 25:28:36:GLU:H    | 1.63                     | 0.64              |
| 32:B:117:GLU:O     | 32:B:121:GLN:HG3  | 1.98                     | 0.64              |
| 35:E:107:GLY:CA    | 53:A:9:G:H5'      | 2.25                     | 0.64              |
| 35:E:149:PRO:HA    | 35:E:152:VAL:HG22 | 1.80                     | 0.64              |
| 41:K:34:THR:HA     | 41:K:41:LEU:HG    | 1.80                     | 0.64              |
| 44:N:27:LYS:O      | 44:N:31:SER:HB2   | 1.98                     | 0.64              |
| 51:U:14:ALA:HB1    | 51:U:16:ARG:HG2   | 1.80                     | 0.64              |
| 53:A:667:G:H2'     | 53:A:668:G:H8     | 1.63                     | 0.64              |
| 54:01:69:C:O2'     | 54:01:70:G:H5'    | 1.98                     | 0.64              |
| 54:01:2039:U:H2'   | 54:01:2040:G:H8   | 1.62                     | 0.64              |
| 16:19:93:ILE:O     | 16:19:97:ILE:HG13 | 1.98                     | 0.63              |
| 34:D:143:SER:C     | 34:D:144:ILE:HD12 | 2.23                     | 0.63              |
| 36:F:51:ILE:HD11   | 48:R:65:SER:HB2   | 1.79                     | 0.63              |
| 54:01:2799:A:H2'   | 54:01:2800:A:H5'  | 1.80                     | 0.63              |
| 4:07:116:LEU:HD22  | 4:07:174:PHE:HB3  | 1.79                     | 0.63              |
| 6:09:9:VAL:HB      | 6:09:13:GLY:CA    | 2.29                     | 0.63              |
| 18:21:57:ASN:OD1   | 54:01:495:G:H1'   | 1.97                     | 0.63              |
| 35:E:98:ALA:HB2    | 35:E:123:LEU:HG   | 1.81                     | 0.63              |
| 54:01:2423:U:O2'   | 54:01:2425:A:H2'  | 1.98                     | 0.63              |
| 54:01:2537:U:H2'   | 54:01:2538:C:C6   | 2.34                     | 0.63              |
| 53:A:501:C:H2'     | 53:A:502:A:C8     | 2.33                     | 0.63              |
| 54:01:441:U:O2'    | 54:01:442:G:H5'   | 1.98                     | 0.63              |
| 54:01:1872:A:H2'   | 54:01:1873:G:O4'  | 1.98                     | 0.63              |
| 54:01:2508:G:H1    | 54:01:2580:U:H3   | 1.44                     | 0.63              |
| 1:04:140:VAL:HG12  | 1:04:191:LEU:HD23 | 1.81                     | 0.63              |
| 2:05:135:GLY:HA2   | 54:01:743:A:OP1   | 1.98                     | 0.63              |
| 4:07:134:GLN:HB3   | 4:07:149:ARG:O    | 1.99                     | 0.63              |
| 11:14:101:ILE:HG13 | 11:14:102:GLY:N   | 2.11                     | 0.63              |
| 43:M:15:VAL:HG23   | 43:M:16:ILE:CD1   | 2.26                     | 0.63              |
| 1:04:30:ALA:HB3    | 1:04:31:PRO:HD3   | 1.81                     | 0.63              |
| 9:12:117:ALA:HA    | 9:12:120:ARG:NH2  | 2.12                     | 0.63              |
| 16:19:40:LYS:HE3   | 54:01:563:A:H4'   | 1.79                     | 0.63              |
| 18:21:51:LEU:O     | 18:21:55:ILE:HG13 | 1.97                     | 0.63              |
| 34:D:7:LYS:NZ      | 34:D:21:LYS:HG3   | 2.14                     | 0.63              |
| 54:01:679:C:H2'    | 54:01:680:C:H6    | 1.62                     | 0.63              |
| 17:20:81:LYS:HD2   | 54:01:973:A:H5''  | 1.80                     | 0.63              |
| 33:C:76:ILE:HB     | 33:C:80:GLY:HA2   | 1.79                     | 0.63              |
| 40:J:10:LEU:CD1    | 40:J:72:ARG:HB2   | 2.27                     | 0.63              |
| 47:Q:44:HIS:O      | 47:Q:70:LYS:HA    | 1.98                     | 0.63              |
| 53:A:225:C:C3'     | 53:A:226:G:H5''   | 2.29                     | 0.63              |
| 22:25:33:ILE:HG22  | 22:25:34:VAL:HG23 | 1.81                     | 0.63              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:E:133:ILE:HD12 | 35:E:133:ILE:N     | 2.11                     | 0.63              |
| 36:F:5:GLU:HA     | 36:F:63:ASN:HA     | 1.79                     | 0.63              |
| 43:M:91:ARG:HD2   | 54:01:888:C:C5     | 2.34                     | 0.63              |
| 46:P:33:ILE:N     | 46:P:33:ILE:HD12   | 2.14                     | 0.63              |
| 52:03:10:VAL:O    | 52:03:14:LYS:HG3   | 1.99                     | 0.63              |
| 53:A:211:G:C2'    | 53:A:212:G:H5'     | 2.28                     | 0.63              |
| 54:01:1026:G:H2'  | 54:01:1027:A:H8    | 1.64                     | 0.63              |
| 38:H:95:MET:SD    | 38:H:129:ALA:HB1   | 2.39                     | 0.63              |
| 54:01:2743:U:C3'  | 54:01:2744:G:H5''  | 2.28                     | 0.63              |
| 1:04:239:PHE:O    | 1:04:241:LYS:HG3   | 1.99                     | 0.63              |
| 3:06:128:ALA:C    | 3:06:156:ASN:HD21  | 2.07                     | 0.63              |
| 41:K:49:SER:OG    | 41:K:68:ARG:HD3    | 1.99                     | 0.63              |
| 54:01:774:G:O2'   | 54:01:775:G:H5''   | 1.99                     | 0.63              |
| 1:04:116:GLN:HE21 | 1:04:121:ALA:CA    | 2.12                     | 0.62              |
| 13:16:2:ARG:HD2   | 54:01:1653:G:H3'   | 1.80                     | 0.62              |
| 22:25:38:GLY:HA2  | 54:01:2330:G:H21   | 1.62                     | 0.62              |
| 38:H:9:MET:HG3    | 38:H:26:MET:SD     | 2.39                     | 0.62              |
| 49:S:27:LYS:HG2   | 49:S:28:LYS:N      | 2.10                     | 0.62              |
| 52:03:5:THR:O     | 52:03:9:ARG:HG3    | 1.98                     | 0.62              |
| 10:13:13:ASN:HD21 | 10:13:98:ARG:HB2   | 1.64                     | 0.62              |
| 14:17:11:ALA:O    | 14:17:15:ARG:HG2   | 1.99                     | 0.62              |
| 33:C:35:ASP:O     | 33:C:38:VAL:HG22   | 1.99                     | 0.62              |
| 35:E:13:LYS:HE2   | 35:E:115:GLU:OE2   | 1.98                     | 0.62              |
| 54:01:2130:U:H5'  | 54:01:2159:G:N2    | 2.13                     | 0.62              |
| 5:08:71:LEU:HA    | 5:08:74:MET:HB2    | 1.80                     | 0.62              |
| 11:14:110:VAL:HB  | 11:14:127:VAL:HG13 | 1.82                     | 0.62              |
| 13:16:79:LEU:CD2  | 13:16:83:LEU:HD12  | 2.30                     | 0.62              |
| 15:18:90:ALA:HB2  | 15:18:112:ARG:HB2  | 1.80                     | 0.62              |
| 42:L:2:THR:CG2    | 42:L:5:GLN:HG3     | 2.29                     | 0.62              |
| 42:L:39:THR:HG22  | 42:L:40:THR:N      | 2.13                     | 0.62              |
| 42:L:51:VAL:HG23  | 42:L:64:SER:O      | 1.99                     | 0.62              |
| 5:08:82:PHE:CE2   | 5:08:137:LYS:HB2   | 2.34                     | 0.62              |
| 8:11:118:GLY:HA3  | 8:11:124:MET:HG2   | 1.81                     | 0.62              |
| 9:12:36:LEU:O     | 9:12:51:GLY:HA3    | 1.99                     | 0.62              |
| 14:17:70:ALA:O    | 14:17:74:VAL:HG23  | 2.00                     | 0.62              |
| 17:20:51:VAL:HB   | 17:20:52:PRO:HD2   | 1.81                     | 0.62              |
| 19:22:51:PHE:O    | 19:22:53:VAL:HG13  | 2.00                     | 0.62              |
| 36:F:12:PRO:HG2   | 36:F:54:LEU:HD21   | 1.80                     | 0.62              |
| 49:S:62:THR:HG22  | 49:S:63:ASP:N      | 2.11                     | 0.62              |
| 53:A:1280:A:O2'   | 53:A:1281:C:H5'    | 2.00                     | 0.62              |
| 54:01:1368:G:H2'  | 54:01:1369:G:H8    | 1.64                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 54:01:2743:U:H2'  | 54:01:2744:G:H5''  | 1.81                     | 0.62              |
| 7:10:97:LYS:HE2   | 7:10:127:ALA:HA    | 1.81                     | 0.62              |
| 28:31:4:ILE:HD12  | 28:31:4:ILE:N      | 2.13                     | 0.62              |
| 34:D:66:VAL:HG12  | 34:D:67:LEU:N      | 2.13                     | 0.62              |
| 42:L:23:LEU:HG    | 42:L:24:GLU:H      | 1.64                     | 0.62              |
| 54:01:2329:U:H2'  | 54:01:2330:G:H8    | 1.64                     | 0.62              |
| 24:27:42:LEU:O    | 24:27:46:VAL:HG23  | 1.99                     | 0.62              |
| 36:F:12:PRO:O     | 36:F:15:SER:HB3    | 1.99                     | 0.62              |
| 41:K:43:TRP:HZ3   | 41:K:45:THR:HG23   | 1.64                     | 0.62              |
| 54:01:1972:G:H2'  | 54:01:1973:G:H8    | 1.65                     | 0.62              |
| 1:04:48:ILE:HD11  | 1:04:51:ARG:HA     | 1.80                     | 0.62              |
| 1:04:229:HIS:ND1  | 1:04:230:PRO:HD2   | 2.15                     | 0.62              |
| 8:11:34:ILE:HD12  | 8:11:34:ILE:N      | 2.14                     | 0.62              |
| 13:16:44:LEU:HD23 | 13:16:113:ILE:HD13 | 1.80                     | 0.62              |
| 36:F:7:VAL:HG22   | 36:F:61:LEU:HD13   | 1.80                     | 0.62              |
| 3:06:163:ASN:HB2  | 54:01:322:A:OP2    | 2.00                     | 0.62              |
| 8:11:93:ASN:HD22  | 54:01:1077:A:H4'   | 1.64                     | 0.62              |
| 13:16:24:MET:HE3  | 13:16:44:LEU:HD22  | 1.80                     | 0.62              |
| 20:23:32:LYS:HB3  | 20:23:63:ALA:HB1   | 1.80                     | 0.62              |
| 32:B:15:PHE:CB    | 59:Z:43:LYS:HB2    | 2.29                     | 0.62              |
| 34:D:144:ILE:HD12 | 34:D:144:ILE:N     | 2.14                     | 0.62              |
| 34:D:164:ARG:HG2  | 34:D:165:GLU:H     | 1.65                     | 0.62              |
| 41:K:111:ASP:OD1  | 41:K:113:THR:HG23  | 2.00                     | 0.62              |
| 52:03:4:LEU:HD12  | 52:03:12:ARG:CD    | 2.29                     | 0.62              |
| 35:E:35:LEU:HD22  | 35:E:133:ILE:HG13  | 1.80                     | 0.62              |
| 35:E:75:LEU:O     | 35:E:75:LEU:HD12   | 1.99                     | 0.62              |
| 1:04:200:MET:HE3  | 53:A:773:G:H4'     | 1.81                     | 0.62              |
| 7:10:94:ARG:O     | 7:10:98:GLU:HG2    | 2.00                     | 0.62              |
| 13:16:33:ILE:HD12 | 13:16:118:ARG:NH2  | 2.14                     | 0.62              |
| 20:23:4:ILE:HD12  | 20:23:4:ILE:H      | 1.65                     | 0.62              |
| 35:E:15:ILE:HD13  | 35:E:36:THR:HA     | 1.82                     | 0.62              |
| 35:E:88:HIS:CE1   | 35:E:89:THR:HG1    | 2.18                     | 0.62              |
| 44:N:92:ILE:HD12  | 44:N:92:ILE:N      | 2.12                     | 0.62              |
| 1:04:106:PRO:HD2  | 1:04:109:LEU:HD22  | 1.81                     | 0.61              |
| 3:06:23:PHE:N     | 3:06:114:ARG:HH22  | 1.98                     | 0.61              |
| 15:18:105:LYS:O   | 15:18:108:ARG:HG2  | 2.00                     | 0.61              |
| 18:21:74:ILE:HG23 | 18:21:74:ILE:O     | 2.00                     | 0.61              |
| 33:C:161:ILE:C    | 33:C:161:ILE:HD12  | 2.25                     | 0.61              |
| 37:G:36:SER:HA    | 39:I:42:THR:HG21   | 1.81                     | 0.61              |
| 52:03:66:PRO:HD2  | 52:03:188:ASN:OD1  | 2.00                     | 0.61              |
| 3:06:40:ARG:HD2   | 54:01:443:A:C6     | 2.35                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:07:90:LEU:HD13  | 4:07:95:MET:HA    | 1.82                     | 0.61              |
| 8:11:11:GLN:HB2   | 8:11:56:VAL:HG12  | 1.81                     | 0.61              |
| 14:17:18:LEU:HD21 | 14:17:25:ARG:HB2  | 1.81                     | 0.61              |
| 19:22:32:LEU:HD12 | 19:22:32:LEU:O    | 2.00                     | 0.61              |
| 33:C:107:LYS:HD3  | 33:C:110:LEU:HD12 | 1.80                     | 0.61              |
| 40:J:10:LEU:HD12  | 40:J:10:LEU:O     | 2.00                     | 0.61              |
| 54:01:1367:A:H2'  | 54:01:1368:G:H5'  | 1.82                     | 0.61              |
| 1:04:69:ASN:HA    | 1:04:188:ARG:HH12 | 1.66                     | 0.61              |
| 5:08:100:ASN:HA   | 5:08:116:LEU:HD12 | 1.82                     | 0.61              |
| 23:26:65:THR:O    | 23:26:69:GLU:HG3  | 2.00                     | 0.61              |
| 33:C:109:GLU:HB2  | 33:C:143:LEU:CD2  | 2.30                     | 0.61              |
| 34:D:100:VAL:HG21 | 34:D:136:VAL:HG21 | 1.81                     | 0.61              |
| 53:A:452:A:H61    | 53:A:480:U:H3     | 1.48                     | 0.61              |
| 53:A:918:A:H2'    | 53:A:919:A:C8     | 2.35                     | 0.61              |
| 54:01:1657:U:H2'  | 54:01:1658:C:C6   | 2.35                     | 0.61              |
| 2:05:8:LYS:HB2    | 2:05:201:LEU:HD11 | 1.80                     | 0.61              |
| 32:B:96:LEU:O     | 32:B:99:MET:HG3   | 1.99                     | 0.61              |
| 35:E:15:ILE:HD12  | 35:E:15:ILE:N     | 2.15                     | 0.61              |
| 38:H:54:THR:C     | 38:H:56:PRO:HD3   | 2.26                     | 0.61              |
| 41:K:59:PRO:HD3   | 41:K:90:PRO:HB2   | 1.80                     | 0.61              |
| 54:01:575:A:O2'   | 54:01:576:U:H5'   | 2.00                     | 0.61              |
| 54:01:2248:C:C2'  | 54:01:2249:U:H5'  | 2.31                     | 0.61              |
| 3:06:1:MET:N      | 3:06:14:VAL:O     | 2.33                     | 0.61              |
| 15:18:29:VAL:CG1  | 15:18:79:VAL:HG22 | 2.30                     | 0.61              |
| 24:27:1:MET:HA    | 24:27:4:LYS:NZ    | 2.15                     | 0.61              |
| 27:30:10:SER:O    | 27:30:14:MET:HG3  | 1.99                     | 0.61              |
| 38:H:64:TYR:HD1   | 38:H:69:ALA:HA    | 1.65                     | 0.61              |
| 40:J:39:PRO:HA    | 40:J:73:LEU:O     | 1.99                     | 0.61              |
| 44:N:27:LYS:HE2   | 53:A:1317:C:OP2   | 2.00                     | 0.61              |
| 54:01:2243:U:H2'  | 54:01:2244:U:C6   | 2.34                     | 0.61              |
| 8:11:38:CYS:O     | 8:11:41:PHE:HB3   | 2.01                     | 0.61              |
| 29:32:1:MET:HG3   | 29:32:1:MET:O     | 1.99                     | 0.61              |
| 46:P:66:THR:C     | 46:P:67:ILE:HD12  | 2.25                     | 0.61              |
| 54:01:2818:U:H2'  | 54:01:2819:G:H8   | 1.66                     | 0.61              |
| 32:B:134:LEU:HG   | 32:B:138:ARG:NE   | 2.14                     | 0.61              |
| 35:E:111:ARG:HH11 | 35:E:111:ARG:HG3  | 1.65                     | 0.61              |
| 44:N:8:ARG:HG2    | 44:N:12:ARG:NH1   | 2.14                     | 0.61              |
| 3:06:7:ASP:CG     | 3:06:8:ALA:H      | 2.09                     | 0.61              |
| 6:09:27:ARG:NH1   | 23:26:55:MET:HB3  | 2.15                     | 0.61              |
| 8:11:11:GLN:HB2   | 8:11:56:VAL:CG1   | 2.29                     | 0.61              |
| 35:E:14:LEU:HA    | 35:E:36:THR:HG22  | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:A:1237:C:OP1   | 53:A:1238:A:H1'   | 2.00                     | 0.61              |
| 54:01:310:A:O2'   | 54:01:311:A:H5''  | 2.01                     | 0.61              |
| 3:06:104:ALA:O    | 3:06:108:ILE:HG13 | 2.01                     | 0.61              |
| 9:12:101:ILE:HD12 | 9:12:101:ILE:N    | 2.15                     | 0.61              |
| 14:17:29:HIS:CE1  | 55:02:7:G:H5'     | 2.36                     | 0.61              |
| 16:19:80:ASN:ND2  | 16:19:84:LYS:HE3  | 2.16                     | 0.61              |
| 37:G:30:MET:HE1   | 53:A:1373:G:O2'   | 2.01                     | 0.61              |
| 42:L:109:ARG:HB2  | 42:L:118:VAL:HG21 | 1.82                     | 0.61              |
| 44:N:80:ARG:O     | 44:N:83:VAL:HG12  | 2.01                     | 0.61              |
| 53:A:346:G:H2'    | 53:A:347:G:H5'    | 1.81                     | 0.61              |
| 53:A:1540:U:O2    | 53:A:1540:U:H3'   | 2.01                     | 0.61              |
| 54:01:1001:A:H2'  | 54:01:1002:G:O4'  | 2.01                     | 0.61              |
| 2:05:122:VAL:HG21 | 2:05:141:ARG:HB3  | 1.83                     | 0.61              |
| 8:11:36:GLU:HA    | 8:11:39:LYS:HB2   | 1.82                     | 0.61              |
| 16:19:56:PHE:CE2  | 54:01:536:G:H4'   | 2.36                     | 0.61              |
| 23:26:11:PRO:HG3  | 23:26:30:PRO:HD2  | 1.82                     | 0.61              |
| 35:E:82:HIS:HB2   | 35:E:83:PRO:HD2   | 1.82                     | 0.61              |
| 52:03:6:LYS:HD2   | 54:01:2132:U:H5   | 1.65                     | 0.61              |
| 54:01:1570:A:H2'  | 54:01:1571:A:C8   | 2.36                     | 0.61              |
| 54:01:2039:U:H2'  | 54:01:2040:G:C8   | 2.35                     | 0.61              |
| 8:11:101:SER:HB3  | 8:11:104:GLN:HG3  | 1.82                     | 0.60              |
| 13:16:73:ASN:O    | 13:16:76:VAL:HG12 | 2.01                     | 0.60              |
| 25:28:40:THR:OG1  | 25:28:41:PRO:HD2  | 2.01                     | 0.60              |
| 32:B:39:ILE:HG22  | 32:B:40:ILE:H     | 1.66                     | 0.60              |
| 34:D:32:LYS:HG3   | 53:A:413:G:O6     | 2.01                     | 0.60              |
| 53:A:328:C:H5'    | 53:A:329:A:H5'    | 1.83                     | 0.60              |
| 54:01:1105:U:C2'  | 54:01:1106:G:H5'' | 2.30                     | 0.60              |
| 5:08:66:THR:OG1   | 54:01:2748:A:H1'  | 1.99                     | 0.60              |
| 7:10:29:ASP:HB3   | 7:10:32:GLY:HA3   | 1.84                     | 0.60              |
| 9:12:21:THR:HA    | 9:12:61:LYS:HB3   | 1.82                     | 0.60              |
| 21:24:10:LYS:HG3  | 21:24:11:GLU:H    | 1.67                     | 0.60              |
| 25:28:35:VAL:HG22 | 25:28:36:GLU:N    | 2.16                     | 0.60              |
| 38:H:76:ARG:NH1   | 38:H:125:ILE:HG23 | 2.17                     | 0.60              |
| 39:I:33:SER:HB3   | 39:I:36:GLN:HG2   | 1.83                     | 0.60              |
| 43:M:48:SER:HB2   | 43:M:51:GLN:HG3   | 1.83                     | 0.60              |
| 48:R:12:PHE:C     | 48:R:14:ALA:H     | 2.09                     | 0.60              |
| 1:04:153:LEU:HD11 | 1:04:181:ARG:HH22 | 1.66                     | 0.60              |
| 6:09:132:PHE:HB2  | 6:09:140:ALA:HB3  | 1.82                     | 0.60              |
| 37:G:78:ARG:HB3   | 37:G:83:THR:HG23  | 1.83                     | 0.60              |
| 53:A:946:A:H2'    | 53:A:947:G:C8     | 2.35                     | 0.60              |
| 27:30:9:ARG:HG3   | 27:30:9:ARG:HH21  | 1.67                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:D:27:ILE:HD12  | 34:D:27:ILE:N     | 2.16                     | 0.60              |
| 36:F:15:SER:HA    | 36:F:18:VAL:HG23  | 1.83                     | 0.60              |
| 37:G:138:GLU:O    | 37:G:142:ARG:HG2  | 2.01                     | 0.60              |
| 38:H:55:LYS:HE3   | 53:A:653:U:H1'    | 1.84                     | 0.60              |
| 44:N:26:LEU:HD23  | 44:N:47:LEU:CD1   | 2.31                     | 0.60              |
| 51:U:32:ARG:HG3   | 51:U:33:ARG:HG2   | 1.84                     | 0.60              |
| 53:A:1230:C:H5'   | 56:W:30:G:H5''    | 1.83                     | 0.60              |
| 54:01:633:A:H2'   | 54:01:634:C:H5'   | 1.82                     | 0.60              |
| 40:J:70:HIS:C     | 40:J:71:LEU:HD12  | 2.26                     | 0.60              |
| 53:A:516:U:H3     | 53:A:533:A:H62    | 1.50                     | 0.60              |
| 54:01:1447:C:H2'  | 54:01:1448:G:H8   | 1.65                     | 0.60              |
| 6:09:117:LEU:N    | 6:09:118:PRO:HD3  | 2.17                     | 0.60              |
| 37:G:111:GLY:HA2  | 37:G:118:ARG:HH11 | 1.66                     | 0.60              |
| 46:P:29:ASN:N     | 46:P:29:ASN:HD22  | 1.98                     | 0.60              |
| 52:03:7:ARG:O     | 52:03:11:ILE:HG13 | 2.01                     | 0.60              |
| 53:A:1512:U:H2'   | 53:A:1513:A:H8    | 1.65                     | 0.60              |
| 54:01:473:G:O2'   | 54:01:474:G:H5'   | 2.01                     | 0.60              |
| 54:01:2389:G:H5'' | 54:01:2390:U:O4'  | 2.02                     | 0.60              |
| 8:11:128:ILE:N    | 8:11:128:ILE:HD12 | 2.16                     | 0.60              |
| 9:12:93:ILE:HG23  | 9:12:97:PRO:HB3   | 1.83                     | 0.60              |
| 26:29:44:PHE:CE1  | 26:29:45:THR:HG23 | 2.37                     | 0.60              |
| 33:C:13:ILE:HD11  | 53:A:1113:C:H4'   | 1.82                     | 0.60              |
| 35:E:14:LEU:C     | 35:E:15:ILE:HD12  | 2.26                     | 0.60              |
| 50:T:23:ARG:HH22  | 50:T:63:LYS:HZ2   | 1.48                     | 0.60              |
| 53:A:112:G:N2     | 53:A:354:G:H5'    | 2.16                     | 0.60              |
| 53:A:667:G:H2'    | 53:A:668:G:C8     | 2.36                     | 0.60              |
| 53:A:1033:G:C2'   | 53:A:1034:G:H5''  | 2.29                     | 0.60              |
| 54:01:2553:G:C3'  | 54:01:2554:U:H5'' | 2.31                     | 0.60              |
| 56:X:69:C:H2'     | 56:X:70:G:H5'     | 1.84                     | 0.60              |
| 11:14:79:LEU:HG   | 11:14:111:ILE:O   | 2.00                     | 0.60              |
| 15:18:3:ILE:H     | 15:18:3:ILE:CD1   | 2.15                     | 0.60              |
| 18:21:29:VAL:HG23 | 18:21:69:LEU:O    | 2.01                     | 0.60              |
| 46:P:67:ILE:HD12  | 46:P:67:ILE:N     | 2.16                     | 0.60              |
| 53:A:346:G:C2'    | 53:A:347:G:H5'    | 2.32                     | 0.60              |
| 54:01:581:C:H2'   | 54:01:582:A:C8    | 2.37                     | 0.60              |
| 24:27:52:ARG:NH2  | 24:27:52:ARG:HB2  | 2.16                     | 0.60              |
| 32:B:72:LYS:HZ1   | 32:B:204:ASP:HA   | 1.65                     | 0.60              |
| 33:C:62:SER:HA    | 33:C:97:PRO:HG2   | 1.83                     | 0.60              |
| 38:H:28:SER:HB3   | 38:H:56:PRO:HB2   | 1.83                     | 0.60              |
| 40:J:15:HIS:HB3   | 40:J:70:HIS:CE1   | 2.36                     | 0.60              |
| 42:L:113:ARG:HE   | 42:L:120:ARG:HA   | 1.67                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:Q:28:VAL:HG22   | 47:Q:29:LYS:N      | 2.17                     | 0.60              |
| 48:R:12:PHE:CD2    | 48:R:13:THR:HG22   | 2.36                     | 0.60              |
| 50:T:82:ILE:HG13   | 50:T:83:ASN:N      | 2.17                     | 0.60              |
| 54:01:582:A:H2'    | 54:01:583:G:C8     | 2.36                     | 0.60              |
| 2:05:148:GLN:HE22  | 2:05:156:PHE:HE2   | 1.49                     | 0.60              |
| 10:13:77:ILE:HG12  | 15:18:71:ARG:HG3   | 1.82                     | 0.60              |
| 16:19:40:LYS:HG2   | 16:19:44:TYR:CE2   | 2.37                     | 0.60              |
| 20:23:82:VAL:HG12  | 20:23:83:GLY:N     | 2.13                     | 0.60              |
| 32:B:216:VAL:O     | 32:B:220:VAL:HG23  | 2.01                     | 0.60              |
| 48:R:13:THR:O      | 48:R:17:VAL:N      | 2.35                     | 0.60              |
| 53:A:31:G:H5'      | 53:A:306:A:C2      | 2.37                     | 0.60              |
| 1:04:116:GLN:NE2   | 1:04:121:ALA:HA    | 2.16                     | 0.59              |
| 4:07:102:LEU:HA    | 4:07:106:ALA:HB3   | 1.84                     | 0.59              |
| 5:08:36:LEU:HD22   | 5:08:67:ALA:HB1    | 1.84                     | 0.59              |
| 42:L:74:GLN:O      | 42:L:76:HIS:N      | 2.32                     | 0.59              |
| 44:N:20:PHE:O      | 44:N:21:ALA:HB3    | 2.02                     | 0.59              |
| 53:A:252:U:O2      | 53:A:252:U:H2'     | 2.01                     | 0.59              |
| 54:01:215:G:C4'    | 54:01:216:A:H4'    | 2.31                     | 0.59              |
| 3:06:134:LEU:HD21  | 3:06:161:ALA:HB2   | 1.83                     | 0.59              |
| 4:07:140:ILE:HD12  | 4:07:140:ILE:N     | 2.18                     | 0.59              |
| 12:15:40:ARG:NH1   | 12:15:73:ILE:HG13  | 2.17                     | 0.59              |
| 15:18:113:LEU:HD12 | 15:18:113:LEU:O    | 2.01                     | 0.59              |
| 16:19:105:PHE:HA   | 16:19:108:LEU:HD12 | 1.84                     | 0.59              |
| 24:27:1:MET:HA     | 24:27:4:LYS:HE2    | 1.84                     | 0.59              |
| 32:B:3:VAL:HG11    | 32:B:211:LEU:HD11  | 1.84                     | 0.59              |
| 33:C:122:GLN:O     | 33:C:127:VAL:HG12  | 2.02                     | 0.59              |
| 52:03:190:GLU:HA   | 52:03:193:LEU:HD12 | 1.83                     | 0.59              |
| 54:01:161:A:H3'    | 54:01:162:U:H5''   | 1.84                     | 0.59              |
| 26:29:46:GLY:HA2   | 26:29:49:ARG:HH21  | 1.67                     | 0.59              |
| 38:H:6:ILE:HG21    | 38:H:76:ARG:NH1    | 2.16                     | 0.59              |
| 46:P:24:SER:HB2    | 53:A:377:G:H5''    | 1.84                     | 0.59              |
| 54:01:2156:G:C2'   | 54:01:2157:G:H5'   | 2.32                     | 0.59              |
| 3:06:24:ASN:HD22   | 3:06:27:LEU:CB     | 2.15                     | 0.59              |
| 10:13:79:PHE:HD1   | 15:18:69:VAL:HG22  | 1.67                     | 0.59              |
| 11:14:70:LYS:O     | 11:14:73:ILE:HG12  | 2.02                     | 0.59              |
| 11:14:77:ILE:HD12  | 11:14:77:ILE:N     | 2.17                     | 0.59              |
| 52:03:8:MET:O      | 52:03:12:ARG:HG3   | 2.03                     | 0.59              |
| 54:01:322:A:H5'    | 54:01:340:A:H1'    | 1.84                     | 0.59              |
| 54:01:1900:A:H1'   | 54:01:1970:A:H2'   | 1.83                     | 0.59              |
| 54:01:2019:A:H2    | 54:01:2035:G:H22   | 1.51                     | 0.59              |
| 1:04:5:CYS:SG      | 1:04:17:LYS:HE2    | 2.43                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:04:129:LEU:HD11 | 1:04:134:ILE:HG12  | 1.84                     | 0.59              |
| 4:07:91:ARG:HA    | 4:07:95:MET:HB3    | 1.85                     | 0.59              |
| 12:15:36:VAL:HG23 | 12:15:128:THR:HA   | 1.82                     | 0.59              |
| 54:01:729:G:H4'   | 54:01:763:G:H5'    | 1.83                     | 0.59              |
| 54:01:825:A:H2'   | 54:01:826:U:C6     | 2.37                     | 0.59              |
| 55:02:55:U:H2'    | 55:02:56:G:C8      | 2.38                     | 0.59              |
| 3:06:6:LYS:HG3    | 3:06:7:ASP:H       | 1.66                     | 0.59              |
| 7:10:24:SER:OG    | 7:10:117:LEU:HD12  | 2.02                     | 0.59              |
| 7:10:29:ASP:H     | 7:10:56:ARG:HH22   | 1.48                     | 0.59              |
| 15:18:96:LEU:HB3  | 15:18:99:LEU:HD13  | 1.83                     | 0.59              |
| 41:K:43:TRP:CZ3   | 41:K:45:THR:HG23   | 2.37                     | 0.59              |
| 41:K:121:ARG:HG3  | 51:U:35:GLU:OE1    | 2.02                     | 0.59              |
| 52:03:26:ALA:HA   | 52:03:29:LEU:HB3   | 1.83                     | 0.59              |
| 53:A:501:C:H2'    | 53:A:502:A:H8      | 1.66                     | 0.59              |
| 54:01:2329:U:H2'  | 54:01:2330:G:C8    | 2.38                     | 0.59              |
| 55:02:3:C:C3'     | 55:02:4:C:H5''     | 2.33                     | 0.59              |
| 10:13:116:ILE:C   | 10:13:116:ILE:HD12 | 2.27                     | 0.59              |
| 34:D:96:ARG:O     | 34:D:100:VAL:HG23  | 2.03                     | 0.59              |
| 39:I:74:GLN:O     | 39:I:78:ILE:HG13   | 2.02                     | 0.59              |
| 45:O:45:HIS:O     | 45:O:46:LYS:HB2    | 2.02                     | 0.59              |
| 53:A:1238:A:H62   | 53:A:1301:U:H3     | 1.49                     | 0.59              |
| 54:01:2210:U:H4'  | 54:01:2211:A:H2    | 1.67                     | 0.59              |
| 56:X:71:C:H2'     | 56:X:72:A:C8       | 2.37                     | 0.59              |
| 59:Z:100:LYS:HB2  | 59:Z:100:LYS:NZ    | 2.17                     | 0.59              |
| 28:31:37:LYS:HB2  | 28:31:48:TYR:CE2   | 2.37                     | 0.59              |
| 29:32:29:GLN:O    | 29:32:32:ALA:HB3   | 2.03                     | 0.59              |
| 47:Q:46:HIS:HA    | 47:Q:70:LYS:HD2    | 1.84                     | 0.59              |
| 50:T:74:HIS:O     | 50:T:78:LEU:HB2    | 2.01                     | 0.59              |
| 53:A:824:G:H2'    | 53:A:825:A:H8      | 1.68                     | 0.59              |
| 54:01:121:G:H4'   | 54:01:149:A:H5'    | 1.84                     | 0.59              |
| 54:01:546:U:H2'   | 54:01:547:A:H4'    | 1.84                     | 0.59              |
| 17:20:49:ILE:HG22 | 17:20:54:VAL:N     | 2.18                     | 0.59              |
| 37:G:42:VAL:O     | 37:G:46:LEU:HD13   | 2.02                     | 0.59              |
| 53:A:102:G:H2'    | 53:A:103:U:C6      | 2.38                     | 0.59              |
| 54:01:254:G:C2'   | 54:01:255:A:H5''   | 2.32                     | 0.59              |
| 59:Z:130:PHE:C    | 59:Z:131:LEU:HD12  | 2.26                     | 0.59              |
| 13:16:47:VAL:C    | 13:16:50:PRO:HD2   | 2.27                     | 0.59              |
| 18:21:41:LYS:O    | 18:21:44:ALA:HB3   | 2.03                     | 0.59              |
| 40:J:15:HIS:O     | 40:J:18:ILE:HG22   | 2.03                     | 0.59              |
| 41:K:33:ILE:O     | 41:K:41:LEU:HB2    | 2.02                     | 0.59              |
| 54:01:2837:A:H2'  | 54:01:2838:G:H8    | 1.66                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:08:44:HIS:CG    | 5:08:45:ALA:H      | 2.21                     | 0.58              |
| 6:09:2:GLN:HE22   | 6:09:20:ASN:HB2    | 1.68                     | 0.58              |
| 7:10:56:ARG:H     | 54:01:1084:A:H4'   | 1.68                     | 0.58              |
| 9:12:81:ILE:HG23  | 9:12:82:GLY:N      | 2.15                     | 0.58              |
| 28:31:47:ILE:HD12 | 28:31:47:ILE:N     | 2.18                     | 0.58              |
| 54:01:1965:C:H5'' | 54:01:1966:A:H2'   | 1.84                     | 0.58              |
| 13:16:55:ALA:HA   | 13:16:80:PHE:CE1   | 2.37                     | 0.58              |
| 15:18:79:VAL:HG13 | 15:18:80:VAL:HG13  | 1.85                     | 0.58              |
| 37:G:144:ALA:O    | 37:G:148:LYS:N     | 2.36                     | 0.58              |
| 38:H:14:ARG:HD2   | 53:A:875:U:O2'     | 2.03                     | 0.58              |
| 48:R:59:LYS:HD3   | 53:A:734:G:O2'     | 2.03                     | 0.58              |
| 2:05:149:ASN:O    | 2:05:152:PRO:HD2   | 2.03                     | 0.58              |
| 4:07:7:TYR:OH     | 4:07:29:ARG:HB3    | 2.04                     | 0.58              |
| 8:11:75:ALA:HA    | 8:11:78:LEU:HB2    | 1.85                     | 0.58              |
| 9:12:71:ASP:O     | 9:12:73:VAL:HG23   | 2.02                     | 0.58              |
| 19:22:50:LEU:HD23 | 24:27:26:PHE:CE2   | 2.38                     | 0.58              |
| 25:28:8:GLN:HB3   | 25:28:31:ILE:HA    | 1.85                     | 0.58              |
| 27:30:8:THR:HG21  | 54:01:2020:A:H5'   | 1.84                     | 0.58              |
| 29:32:4:THR:O     | 29:32:5:PHE:HB2    | 2.02                     | 0.58              |
| 33:C:71:ARG:O     | 33:C:75:VAL:HG23   | 2.03                     | 0.58              |
| 34:D:37:PRO:HD2   | 34:D:41:GLY:HA3    | 1.85                     | 0.58              |
| 34:D:195:ASN:ND2  | 34:D:198:LEU:HG    | 2.15                     | 0.58              |
| 35:E:136:VAL:HG13 | 35:E:137:ARG:N     | 2.18                     | 0.58              |
| 39:I:25:GLY:O     | 39:I:27:ILE:HD12   | 2.03                     | 0.58              |
| 46:P:20:VAL:HG23  | 46:P:34:GLU:O      | 2.03                     | 0.58              |
| 52:03:9:ARG:O     | 52:03:13:GLU:HG3   | 2.03                     | 0.58              |
| 53:A:225:C:C2'    | 53:A:226:G:H5''    | 2.33                     | 0.58              |
| 53:A:1527:U:O2'   | 53:A:1528:U:H5'    | 2.04                     | 0.58              |
| 54:01:1062:G:N2   | 54:01:1063:G:H21   | 1.99                     | 0.58              |
| 54:01:2257:U:O2'  | 54:01:2258:C:H5'   | 2.04                     | 0.58              |
| 54:01:2285:C:O2'  | 54:01:2287:A:H1'   | 2.02                     | 0.58              |
| 3:06:147:LEU:HD12 | 3:06:168:ASP:O     | 2.04                     | 0.58              |
| 5:08:86:LEU:HD22  | 5:08:147:LEU:HD12  | 1.85                     | 0.58              |
| 8:11:53:PRO:HB2   | 8:11:77:VAL:HG11   | 1.84                     | 0.58              |
| 17:20:49:ILE:HG22 | 17:20:54:VAL:HA    | 1.86                     | 0.58              |
| 18:21:69:LEU:HG   | 18:21:107:VAL:HG22 | 1.86                     | 0.58              |
| 37:G:71:THR:O     | 37:G:90:VAL:HG12   | 2.02                     | 0.58              |
| 38:H:95:MET:O     | 38:H:98:LEU:HG     | 2.02                     | 0.58              |
| 51:U:17:ARG:HA    | 51:U:20:ARG:HH11   | 1.69                     | 0.58              |
| 51:U:38:GLU:C     | 51:U:40:PRO:HD2    | 2.28                     | 0.58              |
| 53:A:59:A:H1'     | 53:A:354:G:N2      | 2.18                     | 0.58              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 53:A:797:C:H2'    | 53:A:798:U:C6    | 2.38                     | 0.58              |
| 1:04:210:ALA:O    | 1:04:213:ARG:HB3 | 2.03                     | 0.58              |
| 24:27:2:LYS:HG3   | 24:27:3:ALA:N    | 2.15                     | 0.58              |
| 52:03:174:THR:CG2 | 54:01:2124:G:H4' | 2.23                     | 0.58              |
| 54:01:741:U:H2'   | 54:01:742:A:H8   | 1.69                     | 0.58              |
| 54:01:1936:A:H2   | 54:01:1943:U:H3  | 1.50                     | 0.58              |
| 5:08:154:GLU:OE2  | 5:08:156:TYR:HB2 | 2.04                     | 0.58              |
| 17:20:80:ARG:NH2  | 54:01:571:U:H3'  | 2.19                     | 0.58              |
| 18:21:56:ALA:HA   | 18:21:59:GLU:HG2 | 1.84                     | 0.58              |
| 19:22:54:GLU:HB3  | 19:22:88:LYS:HD2 | 1.86                     | 0.58              |
| 38:H:10:LEU:HD22  | 38:H:74:ILE:CD1  | 2.33                     | 0.58              |
| 39:I:114:LYS:H    | 39:I:120:ALA:HA  | 1.68                     | 0.58              |
| 42:L:82:ARG:HD3   | 42:L:97:VAL:HG22 | 1.85                     | 0.58              |
| 56:W:69:C:H2'     | 56:W:70:G:H8     | 1.69                     | 0.58              |
| 59:Z:161:GLN:C    | 59:Z:162:LYS:HE3 | 2.27                     | 0.58              |
| 1:04:216:ARG:HG2  | 1:04:217:PRO:HD2 | 1.85                     | 0.58              |
| 9:12:31:GLU:HG2   | 9:12:142:ILE:CG1 | 2.32                     | 0.58              |
| 9:12:101:ILE:H    | 9:12:101:ILE:CD1 | 2.16                     | 0.58              |
| 12:15:33:LEU:HD12 | 12:15:129:THR:O  | 2.03                     | 0.58              |
| 36:F:3:HIS:O      | 36:F:92:THR:HG22 | 2.04                     | 0.58              |
| 36:F:100:SER:HB3  | 36:F:101:PRO:HD3 | 1.85                     | 0.58              |
| 40:J:37:ARG:HB3   | 40:J:75:ASP:HB3  | 1.84                     | 0.58              |
| 51:U:49:ALA:HA    | 53:A:723:U:O4    | 2.03                     | 0.58              |
| 52:03:54:LYS:HG2  | 52:03:56:ASP:OD1 | 2.03                     | 0.58              |
| 53:A:665:A:C1'    | 53:A:733:G:H1'   | 2.34                     | 0.58              |
| 53:A:811:C:H5     | 53:A:812:G:C6    | 2.21                     | 0.58              |
| 53:A:1218:C:H2'   | 53:A:1219:A:H8   | 1.66                     | 0.58              |
| 3:06:63:LYS:HD3   | 54:01:2443:C:OP1 | 2.04                     | 0.58              |
| 5:08:102:ILE:HD12 | 5:08:114:HIS:HD2 | 1.69                     | 0.58              |
| 53:A:952:U:H2'    | 53:A:953:G:H8    | 1.69                     | 0.58              |
| 2:05:151:THR:HB   | 2:05:152:PRO:CD  | 2.26                     | 0.58              |
| 6:09:75:LEU:HB3   | 6:09:77:THR:HG22 | 1.86                     | 0.58              |
| 8:11:109:ALA:O    | 8:11:113:ALA:N   | 2.37                     | 0.58              |
| 46:P:20:VAL:HG22  | 46:P:21:VAL:N    | 2.19                     | 0.58              |
| 48:R:12:PHE:CG    | 48:R:13:THR:N    | 2.64                     | 0.58              |
| 50:T:82:ILE:HG13  | 50:T:83:ASN:H    | 1.69                     | 0.58              |
| 59:Z:150:LYS:NZ   | 59:Z:150:LYS:HB3 | 2.18                     | 0.58              |
| 5:08:51:PHE:CE2   | 5:08:68:ARG:HA   | 2.38                     | 0.58              |
| 9:12:7:LYS:O      | 9:12:11:VAL:HG23 | 2.03                     | 0.58              |
| 12:15:83:GLY:HA2  | 54:01:2276:G:OP2 | 2.03                     | 0.58              |
| 21:24:77:VAL:HG22 | 21:24:78:GLN:N   | 2.19                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:B:202:ASN:ND2  | 32:B:205:ALA:CB   | 2.63                     | 0.58              |
| 33:C:39:ARG:HH12  | 33:C:54:ILE:HG13  | 1.68                     | 0.58              |
| 34:D:191:SER:O    | 34:D:192:ALA:HB3  | 2.03                     | 0.58              |
| 36:F:40:GLU:CD    | 36:F:61:LEU:HD23  | 2.29                     | 0.58              |
| 54:01:225:C:H2'   | 54:01:226:A:O4'   | 2.03                     | 0.58              |
| 55:02:114:C:H2'   | 55:02:115:A:H8    | 1.69                     | 0.58              |
| 21:24:65:VAL:HG13 | 21:24:68:LYS:HB2  | 1.85                     | 0.57              |
| 24:27:51:ALA:O    | 24:27:55:THR:N    | 2.37                     | 0.57              |
| 30:33:54:LEU:O    | 30:33:58:ILE:HG13 | 2.04                     | 0.57              |
| 38:H:9:MET:HE1    | 38:H:35:ILE:HB    | 1.85                     | 0.57              |
| 41:K:19:VAL:HG11  | 41:K:84:MET:HE2   | 1.85                     | 0.57              |
| 48:R:40:PRO:HG2   | 48:R:43:ILE:HG12  | 1.86                     | 0.57              |
| 54:01:2139:U:H2'  | 54:01:2140:G:C8   | 2.39                     | 0.57              |
| 15:18:91:VAL:HG21 | 15:18:96:LEU:HD11 | 1.84                     | 0.57              |
| 16:19:49:ARG:HG2  | 16:19:49:ARG:HH11 | 1.68                     | 0.57              |
| 18:21:77:ASP:OD1  | 18:21:102:HIS:HB2 | 2.04                     | 0.57              |
| 32:B:162:VAL:HG12 | 32:B:163:ILE:N    | 2.19                     | 0.57              |
| 32:B:202:ASN:CA   | 59:Z:43:LYS:HZ1   | 2.15                     | 0.57              |
| 36:F:89:VAL:HG12  | 36:F:90:MET:N     | 2.17                     | 0.57              |
| 39:I:91:GLU:C     | 39:I:93:LEU:N     | 2.57                     | 0.57              |
| 54:01:2715:C:C3'  | 54:01:2716:C:H5'' | 2.34                     | 0.57              |
| 54:01:2743:U:H3'  | 54:01:2744:G:H5'' | 1.86                     | 0.57              |
| 11:14:33:ARG:CD   | 11:14:40:SER:HA   | 2.35                     | 0.57              |
| 14:17:5:SER:HA    | 14:17:8:ILE:HD12  | 1.85                     | 0.57              |
| 14:17:94:ARG:O    | 14:17:97:PHE:HB2  | 2.05                     | 0.57              |
| 16:19:97:ILE:HD13 | 17:20:40:MET:HE1  | 1.86                     | 0.57              |
| 40:J:22:THR:O     | 40:J:25:ILE:HG22  | 2.04                     | 0.57              |
| 42:L:79:ILE:C     | 42:L:79:ILE:HD12  | 2.29                     | 0.57              |
| 44:N:7:ALA:HA     | 44:N:10:VAL:HG12  | 1.86                     | 0.57              |
| 7:10:67:THR:HB    | 7:10:68:PRO:HD3   | 1.86                     | 0.57              |
| 9:12:8:PRO:HG3    | 9:12:48:VAL:HG13  | 1.86                     | 0.57              |
| 12:15:75:GLU:CB   | 12:15:90:GLU:HG3  | 2.33                     | 0.57              |
| 17:20:49:ILE:HG22 | 17:20:54:VAL:CA   | 2.34                     | 0.57              |
| 18:21:29:VAL:O    | 18:21:32:ALA:HB3  | 2.04                     | 0.57              |
| 32:B:202:ASN:HB2  | 59:Z:43:LYS:NZ    | 2.19                     | 0.57              |
| 34:D:96:ARG:NH1   | 34:D:133:SER:HA   | 2.19                     | 0.57              |
| 51:U:13:VAL:HG22  | 51:U:14:ALA:N     | 2.19                     | 0.57              |
| 54:01:573:U:O2'   | 54:01:574:A:H3'   | 2.04                     | 0.57              |
| 3:06:18:THR:HG23  | 3:06:106:LYS:HG2  | 1.86                     | 0.57              |
| 6:09:103:VAL:O    | 6:09:107:GLY:N    | 2.37                     | 0.57              |
| 10:13:25:LEU:HD12 | 10:13:38:ILE:HG22 | 1.86                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:17:26:LEU:HD13 | 14:17:39:VAL:HG22  | 1.87                     | 0.57              |
| 16:19:49:ARG:HH21 | 17:20:72:VAL:HG13  | 1.68                     | 0.57              |
| 18:21:34:ASP:HB3  | 27:30:27:LEU:HD22  | 1.87                     | 0.57              |
| 21:24:82:TYR:CE1  | 21:24:83:LYS:HG3   | 2.39                     | 0.57              |
| 25:28:37:ARG:NH2  | 54:01:929:U:H4'    | 2.19                     | 0.57              |
| 34:D:90:LEU:HD23  | 34:D:93:LEU:HD12   | 1.86                     | 0.57              |
| 46:P:22:ALA:HA    | 46:P:33:ILE:HD13   | 1.85                     | 0.57              |
| 53:A:1005:A:H2'   | 53:A:1006:G:O4'    | 2.05                     | 0.57              |
| 54:01:2691:C:H2'  | 54:01:2692:G:H8    | 1.69                     | 0.57              |
| 54:01:2825:G:H2'  | 54:01:2826:A:H5'   | 1.87                     | 0.57              |
| 5:08:3:VAL:CG2    | 54:01:2751:G:H4'   | 2.35                     | 0.57              |
| 5:08:71:LEU:O     | 5:08:75:VAL:HG23   | 2.04                     | 0.57              |
| 8:11:79:LEU:HA    | 8:11:82:ALA:HB3    | 1.85                     | 0.57              |
| 31:34:19:ARG:HD2  | 31:34:24:ARG:HD2   | 1.85                     | 0.57              |
| 36:F:51:ILE:HD11  | 48:R:65:SER:CB     | 2.35                     | 0.57              |
| 53:A:10:A:H2'     | 53:A:11:G:H8       | 1.67                     | 0.57              |
| 53:A:224:U:H2'    | 53:A:225:C:C6      | 2.40                     | 0.57              |
| 53:A:304:U:O2'    | 53:A:305:G:H5'     | 2.05                     | 0.57              |
| 53:A:769:G:H4'    | 53:A:1513:A:H4'    | 1.86                     | 0.57              |
| 54:01:937:C:H2'   | 54:01:938:G:H8     | 1.68                     | 0.57              |
| 54:01:1101:U:H2'  | 54:01:1102:C:H6    | 1.69                     | 0.57              |
| 54:01:1447:C:H2'  | 54:01:1448:G:C8    | 2.39                     | 0.57              |
| 55:02:95:U:H2'    | 55:02:96:G:H8      | 1.69                     | 0.57              |
| 1:04:65:ASP:CB    | 1:04:101:ARG:HD3   | 2.34                     | 0.57              |
| 2:05:179:ARG:HB3  | 2:05:188:LEU:HD12  | 1.86                     | 0.57              |
| 7:10:59:LEU:HB3   | 7:10:62:ARG:CB     | 2.35                     | 0.57              |
| 11:14:92:LEU:HD23 | 11:14:125:LEU:HD12 | 1.85                     | 0.57              |
| 17:20:53:PHE:O    | 17:20:54:VAL:C     | 2.47                     | 0.57              |
| 23:26:2:ARG:HD2   | 23:26:29:LEU:HD22  | 1.86                     | 0.57              |
| 24:27:21:LEU:HA   | 24:27:25:GLN:HB3   | 1.86                     | 0.57              |
| 33:C:126:ARG:HG2  | 33:C:126:ARG:HH11  | 1.70                     | 0.57              |
| 34:D:21:LYS:O     | 34:D:22:SER:C      | 2.48                     | 0.57              |
| 34:D:142:VAL:O    | 34:D:179:GLY:N     | 2.36                     | 0.57              |
| 35:E:108:GLY:O    | 35:E:109:ALA:HB3   | 2.05                     | 0.57              |
| 36:F:3:HIS:N      | 36:F:92:THR:HG22   | 2.19                     | 0.57              |
| 52:03:3:LYS:O     | 52:03:4:LEU:HD23   | 2.04                     | 0.57              |
| 53:A:437:U:H2'    | 53:A:438:U:O4'     | 2.04                     | 0.57              |
| 53:A:518:C:H5'    | 53:A:530:G:O4'     | 2.04                     | 0.57              |
| 54:01:2715:C:H2'  | 54:01:2716:C:H5''  | 1.86                     | 0.57              |
| 56:W:69:C:H2'     | 56:W:70:G:C8       | 2.39                     | 0.57              |
| 5:08:90:GLY:HA3   | 5:08:93:TYR:CE2    | 2.40                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:14:38:GLN:HG3  | 54:01:805:G:H5''  | 1.86                     | 0.57              |
| 34:D:10:LEU:HD13  | 34:D:62:ARG:HD2   | 1.87                     | 0.57              |
| 34:D:170:LEU:HD12 | 34:D:170:LEU:O    | 2.04                     | 0.57              |
| 38:H:42:GLU:HG2   | 38:H:100:ILE:HD13 | 1.86                     | 0.57              |
| 42:L:2:THR:HB     | 42:L:5:GLN:OE1    | 2.03                     | 0.57              |
| 53:A:78:A:H2'     | 53:A:79:G:O4'     | 2.05                     | 0.57              |
| 53:A:545:C:O2'    | 53:A:546:A:H5'    | 2.05                     | 0.57              |
| 53:A:1412:C:H2'   | 53:A:1413:A:C8    | 2.39                     | 0.57              |
| 54:01:49:A:H5'    | 54:01:51:G:O4'    | 2.05                     | 0.57              |
| 54:01:1319:C:O2'  | 54:01:1320:C:H5'  | 2.05                     | 0.57              |
| 54:01:2554:U:H2'  | 54:01:2555:U:C6   | 2.39                     | 0.57              |
| 1:04:83:ASP:HB2   | 1:04:90:ILE:CD1   | 2.35                     | 0.57              |
| 12:15:12:MET:HA   | 54:01:910:A:N6    | 2.19                     | 0.57              |
| 13:16:24:MET:HE3  | 13:16:44:LEU:HB2  | 1.86                     | 0.57              |
| 15:18:95:LYS:N    | 15:18:95:LYS:HD2  | 2.20                     | 0.57              |
| 23:26:68:ALA:O    | 23:26:71:ARG:HB3  | 2.04                     | 0.57              |
| 32:B:15:PHE:O     | 59:Z:43:LYS:HG3   | 2.04                     | 0.57              |
| 33:C:156:LEU:HD21 | 33:C:163:ARG:O    | 2.05                     | 0.57              |
| 38:H:120:LEU:HD12 | 38:H:120:LEU:O    | 2.04                     | 0.57              |
| 42:L:38:THR:HA    | 42:L:49:ARG:O     | 2.05                     | 0.57              |
| 48:R:21:ASP:OD2   | 48:R:23:LYS:HB2   | 2.05                     | 0.57              |
| 54:01:1796:U:H2'  | 54:01:1797:G:H8   | 1.68                     | 0.57              |
| 54:01:2328:A:H2'  | 54:01:2329:U:C6   | 2.40                     | 0.57              |
| 59:Z:112:ILE:HG12 | 59:Z:122:VAL:HG22 | 1.86                     | 0.57              |
| 4:07:112:ASP:OD1  | 43:M:65:GLU:HG3   | 2.05                     | 0.57              |
| 4:07:113:PHE:CZ   | 4:07:175:PRO:HG2  | 2.39                     | 0.57              |
| 5:08:16:VAL:HG11  | 5:08:49:LEU:CD1   | 2.35                     | 0.57              |
| 15:18:38:ARG:HG2  | 15:18:39:LEU:N    | 2.19                     | 0.57              |
| 18:21:33:LEU:HD23 | 18:21:51:LEU:HD23 | 1.87                     | 0.57              |
| 27:30:46:GLY:HA3  | 27:30:54:ILE:HG21 | 1.87                     | 0.57              |
| 39:I:15:ALA:O     | 39:I:66:VAL:HG23  | 2.04                     | 0.57              |
| 39:I:79:ARG:HH12  | 39:I:102:PHE:HA   | 1.70                     | 0.57              |
| 39:I:87:MET:HG3   | 39:I:88:GLU:N     | 2.20                     | 0.57              |
| 54:01:184:C:H2'   | 54:01:185:G:H8    | 1.70                     | 0.57              |
| 54:01:669:G:H2'   | 54:01:669:G:N3    | 2.19                     | 0.57              |
| 54:01:2487:G:H2'  | 54:01:2488:G:H8   | 1.70                     | 0.57              |
| 16:19:8:ILE:HD12  | 16:19:8:ILE:C     | 2.30                     | 0.56              |
| 18:21:23:LEU:HD22 | 27:30:23:ALA:HB2  | 1.85                     | 0.56              |
| 33:C:125:ARG:HH11 | 33:C:125:ARG:HB2  | 1.70                     | 0.56              |
| 38:H:54:THR:HG23  | 38:H:55:LYS:HG3   | 1.87                     | 0.56              |
| 38:H:64:TYR:CD1   | 38:H:69:ALA:HA    | 2.40                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:N:45:LEU:HG    | 49:S:12:LEU:HD21   | 1.87                     | 0.56              |
| 47:Q:4:ILE:C      | 47:Q:4:ILE:HD12    | 2.30                     | 0.56              |
| 51:U:16:ARG:NH2   | 51:U:19:LYS:HE2    | 2.20                     | 0.56              |
| 1:04:52:HIS:HA    | 1:04:216:ARG:HB3   | 1.86                     | 0.56              |
| 3:06:24:ASN:ND2   | 3:06:27:LEU:HB2    | 2.17                     | 0.56              |
| 4:07:115:GLY:C    | 4:07:116:LEU:HD12  | 2.31                     | 0.56              |
| 10:13:113:MET:O   | 10:13:116:ILE:HG13 | 2.06                     | 0.56              |
| 16:19:51:GLN:HE22 | 16:19:54:ARG:NH1   | 2.04                     | 0.56              |
| 21:24:20:LEU:HD12 | 21:24:21:ARG:N     | 2.20                     | 0.56              |
| 33:C:109:GLU:HB2  | 33:C:143:LEU:HD22  | 1.86                     | 0.56              |
| 37:G:37:THR:O     | 37:G:41:ILE:HG13   | 2.04                     | 0.56              |
| 39:I:20:ILE:HD11  | 39:I:60:LEU:HD13   | 1.87                     | 0.56              |
| 39:I:94:ARG:HA    | 39:I:97:LEU:HB3    | 1.86                     | 0.56              |
| 51:U:58:LYS:HA    | 51:U:61:ARG:HD3    | 1.86                     | 0.56              |
| 53:A:392:C:H2'    | 53:A:393:A:H8      | 1.69                     | 0.56              |
| 1:04:123:ILE:HG21 | 36:F:80:PHE:CE1    | 2.40                     | 0.56              |
| 2:05:118:PHE:CE1  | 2:05:163:GLY:HA2   | 2.41                     | 0.56              |
| 7:10:28:ALA:HB1   | 7:10:81:LEU:HB3    | 1.86                     | 0.56              |
| 10:13:87:LEU:HD22 | 10:13:92:GLU:O     | 2.05                     | 0.56              |
| 15:18:52:ARG:O    | 15:18:56:SER:N     | 2.38                     | 0.56              |
| 16:19:35:PHE:O    | 16:19:39:ILE:HG13  | 2.05                     | 0.56              |
| 32:B:125:PHE:HE1  | 32:B:136:ARG:HB2   | 1.70                     | 0.56              |
| 36:F:100:SER:H    | 36:F:101:PRO:HD2   | 1.71                     | 0.56              |
| 39:I:79:ARG:NH1   | 39:I:102:PHE:HA    | 2.21                     | 0.56              |
| 40:J:67:ILE:HG22  | 44:N:95:LEU:HA     | 1.86                     | 0.56              |
| 41:K:53:GLY:O     | 41:K:56:LYS:HB3    | 2.06                     | 0.56              |
| 42:L:86:VAL:HG21  | 42:L:89:LEU:HD13   | 1.88                     | 0.56              |
| 43:M:9:PRO:HG3    | 43:M:17:ALA:HB1    | 1.86                     | 0.56              |
| 43:M:104:ASN:O    | 43:M:105:ALA:HB3   | 2.04                     | 0.56              |
| 45:O:64:LYS:HD3   | 53:A:755:G:OP2     | 2.05                     | 0.56              |
| 52:03:7:ARG:HH22  | 52:03:11:ILE:HD11  | 1.70                     | 0.56              |
| 53:A:711:G:O2'    | 53:A:712:A:H5'     | 2.03                     | 0.56              |
| 53:A:924:C:H2'    | 53:A:925:G:C8      | 2.40                     | 0.56              |
| 53:A:960:U:H4'    | 53:A:961:U:O5'     | 2.05                     | 0.56              |
| 53:A:1517:G:H2'   | 53:A:1518:A:H5'    | 1.87                     | 0.56              |
| 54:01:306:U:H3    | 54:01:310:A:H62    | 1.53                     | 0.56              |
| 54:01:502:A:H2'   | 54:01:503:A:H5'    | 1.86                     | 0.56              |
| 54:01:799:G:H5''  | 54:01:800:A:H2'    | 1.87                     | 0.56              |
| 54:01:947:A:H2'   | 54:01:948:C:H6     | 1.68                     | 0.56              |
| 4:07:135:ILE:C    | 4:07:135:ILE:HD12  | 2.30                     | 0.56              |
| 15:18:16:VAL:O    | 15:18:18:SER:N     | 2.37                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:21:4:ILE:HG22  | 18:21:106:VAL:HG22 | 1.88                     | 0.56              |
| 35:E:12:GLU:OE1   | 35:E:63:MET:HE3    | 2.04                     | 0.56              |
| 54:01:1720:U:H2'  | 54:01:1721:G:O4'   | 2.04                     | 0.56              |
| 1:04:216:ARG:CG   | 1:04:217:PRO:HD2   | 2.36                     | 0.56              |
| 16:19:30:VAL:HG13 | 54:01:580:U:O3'    | 2.05                     | 0.56              |
| 31:34:32:LYS:HE3  | 54:01:2478:A:H5'   | 1.87                     | 0.56              |
| 46:P:59:HIS:O     | 46:P:63:GLN:HG2    | 2.05                     | 0.56              |
| 52:03:39:VAL:HG13 | 52:03:179:ASP:OD2  | 2.06                     | 0.56              |
| 53:A:70:U:H2'     | 53:A:94:G:O6       | 2.06                     | 0.56              |
| 54:01:1775:U:H2'  | 54:01:1776:G:O4'   | 2.05                     | 0.56              |
| 6:09:79:THR:CG2   | 6:09:147:VAL:HG21  | 2.36                     | 0.56              |
| 10:13:63:VAL:HG23 | 10:13:64:ARG:N     | 2.20                     | 0.56              |
| 11:14:19:LEU:N    | 11:14:19:LEU:HD12  | 2.21                     | 0.56              |
| 16:19:91:ARG:HG3  | 16:19:91:ARG:NH1   | 2.17                     | 0.56              |
| 33:C:141:MET:HG3  | 33:C:169:GLU:HG2   | 1.88                     | 0.56              |
| 37:G:24:LYS:O     | 37:G:28:ILE:HG13   | 2.06                     | 0.56              |
| 37:G:29:LEU:HD23  | 37:G:29:LEU:C      | 2.30                     | 0.56              |
| 41:K:51:PHE:CE2   | 41:K:64:VAL:HG11   | 2.41                     | 0.56              |
| 45:O:87:ARG:O     | 45:O:88:ARG:C      | 2.48                     | 0.56              |
| 54:01:1060:U:H5'  | 54:01:1062:G:C5'   | 2.35                     | 0.56              |
| 54:01:1796:U:H2'  | 54:01:1797:G:C8    | 2.41                     | 0.56              |
| 3:06:146:VAL:HG12 | 3:06:185:LYS:HB2   | 1.88                     | 0.56              |
| 8:11:34:ILE:O     | 8:11:37:PHE:HB3    | 2.06                     | 0.56              |
| 10:13:109:SER:O   | 10:13:110:GLU:HB3  | 2.05                     | 0.56              |
| 15:18:88:ARG:NE   | 15:18:112:ARG:HH21 | 2.04                     | 0.56              |
| 29:32:26:ASN:CG   | 54:01:682:G:H5'    | 2.30                     | 0.56              |
| 37:G:52:ARG:HH12  | 37:G:121:ASN:ND2   | 2.03                     | 0.56              |
| 44:N:86:ALA:HB1   | 44:N:91:GLU:HB2    | 1.86                     | 0.56              |
| 53:A:1401:G:H2'   | 53:A:1402:C:O4'    | 2.06                     | 0.56              |
| 53:A:1412:C:H2'   | 53:A:1413:A:H8     | 1.71                     | 0.56              |
| 53:A:1484:C:H2'   | 53:A:1485:U:C6     | 2.41                     | 0.56              |
| 54:01:414:C:H2'   | 54:01:415:A:C8     | 2.41                     | 0.56              |
| 54:01:565:C:H2'   | 54:01:566:U:C6     | 2.40                     | 0.56              |
| 54:01:2709:G:H2'  | 54:01:2710:C:C6    | 2.40                     | 0.56              |
| 56:W:31:G:H2'     | 56:W:32:C:H6       | 1.71                     | 0.56              |
| 1:04:120:ASP:HA   | 6:09:91:PHE:CZ     | 2.37                     | 0.56              |
| 4:07:141:ASP:C    | 4:07:143:ASP:H     | 2.14                     | 0.56              |
| 7:10:60:LEU:O     | 7:10:64:VAL:HB     | 2.06                     | 0.56              |
| 53:A:763:G:H2'    | 53:A:764:C:H6      | 1.71                     | 0.56              |
| 54:01:1186:G:H2'  | 54:01:1187:G:O4'   | 2.05                     | 0.56              |
| 6:09:84:ALA:HB2   | 6:09:90:LEU:HD12   | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:20:75:VAL:HG22 | 17:20:86:GLN:OE1  | 2.05                     | 0.56              |
| 53:A:40:C:H2'     | 53:A:41:G:H8      | 1.71                     | 0.56              |
| 53:A:1282:C:H2'   | 53:A:1283:U:C6    | 2.40                     | 0.56              |
| 54:01:752:A:O2'   | 54:01:1781:U:H5'  | 2.06                     | 0.56              |
| 54:01:996:A:H2'   | 54:01:997:G:H8    | 1.71                     | 0.56              |
| 54:01:2281:A:O2'  | 54:01:2282:G:H5'  | 2.06                     | 0.56              |
| 3:06:40:ARG:HD2   | 54:01:443:A:C5    | 2.41                     | 0.56              |
| 6:09:45:GLU:HA    | 6:09:48:GLU:OE2   | 2.06                     | 0.56              |
| 9:12:26:GLY:HA3   | 54:01:1140:C:H5'  | 1.87                     | 0.56              |
| 14:17:40:ILE:HD13 | 55:02:8:C:O2'     | 2.06                     | 0.56              |
| 16:19:80:ASN:HD21 | 16:19:84:LYS:HE3  | 1.71                     | 0.56              |
| 17:20:14:VAL:HG23 | 17:20:20:VAL:HG21 | 1.88                     | 0.56              |
| 26:29:44:PHE:CD1  | 26:29:45:THR:HG23 | 2.40                     | 0.56              |
| 37:G:29:LEU:HD23  | 37:G:29:LEU:O     | 2.05                     | 0.56              |
| 41:K:110:THR:HG22 | 51:U:4:LYS:HG3    | 1.88                     | 0.56              |
| 54:01:576:U:H2'   | 54:01:577:G:C8    | 2.41                     | 0.56              |
| 54:01:1906:G:H3'  | 54:01:1907:G:H5'' | 1.87                     | 0.56              |
| 59:Z:101:ALA:O    | 59:Z:106:GLU:HB2  | 2.06                     | 0.56              |
| 9:12:47:HIS:CE1   | 9:12:48:VAL:HG23  | 2.40                     | 0.55              |
| 16:19:24:TYR:CG   | 16:19:25:GLY:N    | 2.73                     | 0.55              |
| 19:22:40:LYS:HE3  | 54:01:1599:U:OP2  | 2.06                     | 0.55              |
| 32:B:6:ARG:HH22   | 59:Z:8:LEU:HD21   | 1.72                     | 0.55              |
| 33:C:82:ASP:O     | 33:C:86:LEU:HG    | 2.06                     | 0.55              |
| 34:D:130:ASN:HD22 | 53:A:619:U:H3     | 1.52                     | 0.55              |
| 39:I:30:ASN:C     | 39:I:32:ARG:H     | 2.14                     | 0.55              |
| 42:L:28:GLN:O     | 42:L:29:LYS:HD2   | 2.05                     | 0.55              |
| 53:A:235:C:H2'    | 53:A:236:A:C8     | 2.41                     | 0.55              |
| 53:A:1318:A:H2'   | 53:A:1319:A:H5'   | 1.87                     | 0.55              |
| 54:01:873:C:H2'   | 54:01:874:G:C8    | 2.41                     | 0.55              |
| 54:01:2475:C:C2'  | 54:01:2476:A:H5'  | 2.36                     | 0.55              |
| 55:02:88:C:H4'    | 55:02:89:U:OP1    | 2.06                     | 0.55              |
| 3:06:149:ILE:HG23 | 3:06:149:ILE:O    | 2.05                     | 0.55              |
| 5:08:86:LEU:N     | 5:08:86:LEU:HD12  | 2.20                     | 0.55              |
| 7:10:87:GLU:HG2   | 7:10:95:LEU:HD12  | 1.87                     | 0.55              |
| 9:12:37:ARG:HH21  | 9:12:37:ARG:HG3   | 1.71                     | 0.55              |
| 10:13:21:CYS:HA   | 10:13:41:ILE:CG2  | 2.35                     | 0.55              |
| 15:18:29:VAL:HG22 | 15:18:80:VAL:HG12 | 1.87                     | 0.55              |
| 32:B:39:ILE:HG22  | 32:B:40:ILE:N     | 2.21                     | 0.55              |
| 34:D:145:ARG:HD2  | 34:D:147:LYS:NZ   | 2.20                     | 0.55              |
| 35:E:52:ALA:HB3   | 35:E:58:ALA:HB2   | 1.89                     | 0.55              |
| 43:M:68:LEU:O     | 43:M:72:ILE:HG13  | 2.06                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:03:52:ALA:CB    | 52:03:167:LYS:HA   | 2.35                     | 0.55              |
| 53:A:1060:U:O2'    | 53:A:1061:G:H5'    | 2.05                     | 0.55              |
| 3:06:32:VAL:HG13   | 3:06:33:VAL:N      | 2.21                     | 0.55              |
| 5:08:34:ARG:NE     | 5:08:70:LEU:HD13   | 2.21                     | 0.55              |
| 7:10:57:ASN:HD22   | 7:10:62:ARG:HG2    | 1.71                     | 0.55              |
| 10:13:116:ILE:HD12 | 10:13:117:SER:N    | 2.22                     | 0.55              |
| 11:14:110:VAL:C    | 11:14:111:ILE:HD12 | 2.31                     | 0.55              |
| 27:30:51:ARG:HB2   | 27:30:51:ARG:HH21  | 1.71                     | 0.55              |
| 34:D:26:ALA:C      | 34:D:27:ILE:HD12   | 2.32                     | 0.55              |
| 35:E:82:HIS:CD2    | 38:H:98:LEU:HD21   | 2.39                     | 0.55              |
| 38:H:50:VAL:O      | 38:H:50:VAL:HG13   | 2.06                     | 0.55              |
| 43:M:54:THR:O      | 43:M:57:ASP:OD1    | 2.24                     | 0.55              |
| 45:O:23:SER:OG     | 45:O:26:VAL:HG23   | 2.06                     | 0.55              |
| 50:T:54:GLN:N      | 50:T:55:PRO:HD2    | 2.22                     | 0.55              |
| 53:A:1418:A:H3'    | 53:A:1419:G:C5'    | 2.35                     | 0.55              |
| 54:01:639:U:H2'    | 54:01:640:C:C6     | 2.41                     | 0.55              |
| 59:Z:159:LEU:HD23  | 59:Z:159:LEU:H     | 1.72                     | 0.55              |
| 1:04:207:ALA:HB2   | 54:01:1790:C:O2'   | 2.07                     | 0.55              |
| 3:06:6:LYS:HG3     | 3:06:7:ASP:N       | 2.21                     | 0.55              |
| 7:10:14:GLU:HA     | 7:10:17:GLU:OE1    | 2.05                     | 0.55              |
| 8:11:128:ILE:HD12  | 8:11:128:ILE:H     | 1.71                     | 0.55              |
| 24:27:1:MET:HA     | 24:27:4:LYS:CE     | 2.37                     | 0.55              |
| 30:33:14:LYS:HD3   | 30:33:22:LYS:CE    | 2.37                     | 0.55              |
| 38:H:46:GLU:O      | 38:H:61:THR:HB     | 2.06                     | 0.55              |
| 41:K:124:LYS:HE2   | 53:A:1524:C:OP2    | 2.05                     | 0.55              |
| 54:01:2055:C:H5'   | 54:01:2056:G:O5'   | 2.06                     | 0.55              |
| 54:01:2183:A:H2'   | 54:01:2184:A:C8    | 2.41                     | 0.55              |
| 3:06:84:THR:HG21   | 54:01:586:A:H5'    | 1.89                     | 0.55              |
| 28:31:46:VAL:HG12  | 28:31:47:ILE:N     | 2.21                     | 0.55              |
| 30:33:33:THR:HG23  | 30:33:34:LYS:N     | 2.21                     | 0.55              |
| 32:B:202:ASN:ND2   | 32:B:205:ALA:HB2   | 2.15                     | 0.55              |
| 32:B:207:ARG:NH2   | 59:Z:41:GLY:HA2    | 2.22                     | 0.55              |
| 37:G:3:ARG:HH22    | 53:A:932:C:H5''    | 1.70                     | 0.55              |
| 37:G:52:ARG:HH12   | 37:G:121:ASN:HD21  | 1.53                     | 0.55              |
| 43:M:1:ALA:N       | 43:M:52:ILE:HD13   | 2.22                     | 0.55              |
| 52:03:44:VAL:HG21  | 52:03:175:ILE:HG23 | 1.89                     | 0.55              |
| 53:A:236:A:H2'     | 53:A:237:G:C8      | 2.41                     | 0.55              |
| 53:A:626:G:H2'     | 53:A:627:G:C8      | 2.41                     | 0.55              |
| 53:A:1255:G:O2'    | 53:A:1258:G:H1'    | 2.06                     | 0.55              |
| 53:A:1432:G:H1'    | 53:A:1468:A:N6     | 2.22                     | 0.55              |
| 54:01:2238:G:N3    | 54:01:2238:G:H2'   | 2.21                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 54:01:2715:C:H3'  | 54:01:2716:C:H5''  | 1.89                     | 0.55              |
| 1:04:260:LYS:O    | 1:04:263:ASP:N     | 2.29                     | 0.55              |
| 4:07:65:LEU:HD22  | 55:02:42:C:C5      | 2.40                     | 0.55              |
| 4:07:103:ILE:HG22 | 4:07:174:PHE:CE1   | 2.41                     | 0.55              |
| 10:13:66:LYS:HG3  | 10:13:81:GLY:O     | 2.07                     | 0.55              |
| 15:18:12:MET:HE3  | 15:18:76:HIS:NE2   | 2.22                     | 0.55              |
| 21:24:42:LEU:HD13 | 21:24:47:VAL:HG21  | 1.88                     | 0.55              |
| 33:C:13:ILE:CD1   | 53:A:1113:C:H4'    | 2.35                     | 0.55              |
| 41:K:35:ASP:OD2   | 41:K:37:GLN:HB2    | 2.06                     | 0.55              |
| 41:K:121:ARG:CZ   | 51:U:35:GLU:HG2    | 2.37                     | 0.55              |
| 42:L:30:ARG:HG2   | 42:L:78:VAL:HG11   | 1.87                     | 0.55              |
| 54:01:1326:U:H2'  | 54:01:1327:A:H8    | 1.70                     | 0.55              |
| 10:13:66:LYS:HD3  | 54:01:1666:G:OP1   | 2.07                     | 0.55              |
| 11:14:90:VAL:HB   | 11:14:122:VAL:HG22 | 1.88                     | 0.55              |
| 12:15:59:ARG:HG3  | 12:15:60:GLN:N     | 2.21                     | 0.55              |
| 13:16:13:ASN:O    | 13:16:14:SER:C     | 2.49                     | 0.55              |
| 16:19:38:VAL:O    | 16:19:41:ALA:HB3   | 2.07                     | 0.55              |
| 43:M:23:GLY:O     | 53:A:1329:A:H4'    | 2.07                     | 0.55              |
| 53:A:715:A:H2'    | 53:A:716:A:H8      | 1.72                     | 0.55              |
| 54:01:2427:C:H5'' | 54:01:2429:G:H5'   | 1.87                     | 0.55              |
| 55:02:95:U:H2'    | 55:02:96:G:C8      | 2.41                     | 0.55              |
| 1:04:253:GLY:O    | 54:01:1844:C:H5'   | 2.07                     | 0.55              |
| 4:07:37:MET:SD    | 4:07:149:ARG:HD3   | 2.47                     | 0.55              |
| 9:12:47:HIS:HD1   | 9:12:48:VAL:HG23   | 1.71                     | 0.55              |
| 15:18:52:ARG:O    | 15:18:53:GLY:C     | 2.49                     | 0.55              |
| 20:23:49:PRO:HA   | 20:23:53:GLN:OE1   | 2.07                     | 0.55              |
| 34:D:7:LYS:HE2    | 53:A:408:A:OP2     | 2.07                     | 0.55              |
| 37:G:21:LEU:HD23  | 37:G:21:LEU:C      | 2.31                     | 0.55              |
| 37:G:92:PRO:O     | 37:G:95:ARG:HB3    | 2.06                     | 0.55              |
| 37:G:140:VAL:O    | 37:G:143:MET:HB2   | 2.07                     | 0.55              |
| 38:H:72:GLU:HB3   | 38:H:129:ALA:OXT   | 2.07                     | 0.55              |
| 38:H:98:LEU:HD12  | 38:H:98:LEU:C      | 2.31                     | 0.55              |
| 40:J:57:VAL:HG22  | 40:J:58:ASN:N      | 2.07                     | 0.55              |
| 42:L:116:TYR:OH   | 53:A:522:C:H5''    | 2.07                     | 0.55              |
| 46:P:33:ILE:HD12  | 46:P:33:ILE:H      | 1.72                     | 0.55              |
| 52:03:21:TYR:CD2  | 52:03:222:VAL:HG13 | 2.42                     | 0.55              |
| 54:01:465:G:C6    | 54:01:466:A:N6     | 2.75                     | 0.55              |
| 6:09:26:ALA:HA    | 6:09:30:LEU:HB2    | 1.86                     | 0.55              |
| 7:10:61:ARG:C     | 7:10:65:GLU:HB2    | 2.31                     | 0.55              |
| 15:18:17:PRO:O    | 15:18:18:SER:C     | 2.50                     | 0.55              |
| 34:D:8:LEU:HD21   | 34:D:31:CYS:HB2    | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:F:32:ALA:CB    | 36:F:70:VAL:HG21  | 2.36                     | 0.55              |
| 48:R:25:ILE:HD12  | 48:R:26:ALA:N     | 2.22                     | 0.55              |
| 54:01:821:A:C5'   | 54:01:822:G:H5''  | 2.33                     | 0.55              |
| 54:01:2105:U:H2'  | 54:01:2106:U:O4'  | 2.07                     | 0.55              |
| 1:04:229:HIS:NE2  | 1:04:246:PRO:HG3  | 2.21                     | 0.55              |
| 13:16:53:THR:O    | 13:16:56:LYS:HG3  | 2.07                     | 0.55              |
| 46:P:2:VAL:HG23   | 46:P:65:ALA:HA    | 1.88                     | 0.55              |
| 50:T:43:LYS:HB3   | 50:T:86:ALA:HB3   | 1.88                     | 0.55              |
| 53:A:1256:A:H1'   | 53:A:1258:G:C5    | 2.42                     | 0.55              |
| 54:01:27:G:N2     | 54:01:512:G:H1'   | 2.22                     | 0.55              |
| 54:01:2141:G:H22  | 54:01:2151:U:H1'  | 1.72                     | 0.55              |
| 4:07:39:VAL:HG12  | 4:07:84:ILE:O     | 2.06                     | 0.54              |
| 7:10:59:LEU:HB3   | 7:10:62:ARG:HB3   | 1.88                     | 0.54              |
| 11:14:17:LYS:HD3  | 54:01:663:G:H5''  | 1.89                     | 0.54              |
| 15:18:92:ARG:O    | 15:18:93:LYS:HB2  | 2.06                     | 0.54              |
| 25:28:23:LEU:HD11 | 25:28:53:MET:SD   | 2.47                     | 0.54              |
| 27:30:45:ASP:O    | 27:30:54:ILE:HG21 | 2.07                     | 0.54              |
| 34:D:71:PHE:HE1   | 34:D:93:LEU:HD21  | 1.72                     | 0.54              |
| 34:D:173:ASP:C    | 34:D:175:GLY:H    | 2.15                     | 0.54              |
| 35:E:44:ARG:HB3   | 35:E:70:MET:HE2   | 1.89                     | 0.54              |
| 38:H:17:GLN:OE1   | 38:H:62:LEU:HD13  | 2.07                     | 0.54              |
| 42:L:46:SER:O     | 42:L:47:ALA:HB2   | 2.06                     | 0.54              |
| 42:L:112:ALA:HB2  | 53:A:503:C:OP2    | 2.07                     | 0.54              |
| 54:01:1213:A:N6   | 54:01:1236:G:H1'  | 2.22                     | 0.54              |
| 54:01:1912:A:H62  | 54:01:1917:U:H3   | 1.53                     | 0.54              |
| 54:01:2623:G:H2'  | 54:01:2624:G:H8   | 1.72                     | 0.54              |
| 59:Z:100:LYS:HB2  | 59:Z:100:LYS:HZ3  | 1.72                     | 0.54              |
| 1:04:86:ARG:HH12  | 54:01:1817:G:C5'  | 2.18                     | 0.54              |
| 4:07:7:TYR:HA     | 4:07:11:VAL:CG2   | 2.37                     | 0.54              |
| 5:08:140:ILE:HG13 | 5:08:141:GLY:N    | 2.21                     | 0.54              |
| 6:09:84:ALA:C     | 6:09:91:PHE:HB2   | 2.32                     | 0.54              |
| 9:12:110:PRO:HB3  | 54:01:1007:C:O3'  | 2.08                     | 0.54              |
| 32:B:16:GLY:HA2   | 59:Z:43:LYS:NZ    | 2.23                     | 0.54              |
| 41:K:57:SER:O     | 41:K:90:PRO:HG3   | 2.07                     | 0.54              |
| 41:K:114:PRO:O    | 41:K:116:PRO:HD3  | 2.06                     | 0.54              |
| 53:A:715:A:H2'    | 53:A:716:A:C8     | 2.42                     | 0.54              |
| 53:A:1199:U:H2'   | 53:A:1200:C:H5'   | 1.87                     | 0.54              |
| 54:01:184:C:H2'   | 54:01:185:G:C8    | 2.42                     | 0.54              |
| 4:07:113:PHE:HZ   | 4:07:175:PRO:HG2  | 1.73                     | 0.54              |
| 5:08:138:GLN:HE22 | 54:01:2759:G:N2   | 2.04                     | 0.54              |
| 7:10:94:ARG:O     | 7:10:97:LYS:HG2   | 2.07                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:25:22:PHE:CD2  | 54:01:922:C:H1'   | 2.43                     | 0.54              |
| 27:30:29:VAL:HG22 | 27:30:36:LYS:HE2  | 1.89                     | 0.54              |
| 38:H:6:ILE:HD11   | 38:H:31:LEU:HD23  | 1.89                     | 0.54              |
| 42:L:113:ARG:HD2  | 42:L:118:VAL:O    | 2.08                     | 0.54              |
| 45:O:25:GLU:H     | 45:O:25:GLU:CD    | 2.14                     | 0.54              |
| 45:O:86:LEU:C     | 45:O:86:LEU:HD12  | 2.33                     | 0.54              |
| 58:Y:44:G:H2'     | 58:Y:45:U:O4'     | 2.07                     | 0.54              |
| 1:04:145:MET:HG2  | 1:04:152:GLN:HG3  | 1.90                     | 0.54              |
| 2:05:77:ARG:HH21  | 2:05:77:ARG:HG3   | 1.71                     | 0.54              |
| 4:07:10:GLU:H     | 4:07:10:GLU:CD    | 2.14                     | 0.54              |
| 4:07:97:GLU:HG2   | 26:29:9:TYR:OH    | 2.07                     | 0.54              |
| 7:10:56:ARG:HB3   | 54:01:1084:A:O4'  | 2.08                     | 0.54              |
| 10:13:6:THR:O     | 10:13:20:MET:HA   | 2.06                     | 0.54              |
| 16:19:93:ILE:HG22 | 16:19:97:ILE:HD11 | 1.89                     | 0.54              |
| 18:21:89:ALA:C    | 18:21:91:GLY:H    | 2.15                     | 0.54              |
| 37:G:87:PRO:HG3   | 37:G:148:LYS:HA   | 1.89                     | 0.54              |
| 42:L:20:VAL:C     | 42:L:22:ALA:H     | 2.16                     | 0.54              |
| 42:L:43:LYS:HB3   | 42:L:44:PRO:CD    | 2.38                     | 0.54              |
| 52:03:4:LEU:HB3   | 52:03:8:MET:HB3   | 1.89                     | 0.54              |
| 54:01:1138:G:H2'  | 54:01:1139:G:O4'  | 2.07                     | 0.54              |
| 54:01:2130:U:H5'  | 54:01:2159:G:H22  | 1.72                     | 0.54              |
| 54:01:2180:U:H4'  | 56:X:17(A):U:O4'  | 2.06                     | 0.54              |
| 2:05:29:VAL:O     | 2:05:185:ASN:HB3  | 2.07                     | 0.54              |
| 19:22:2:ILE:HD11  | 54:01:144:A:H4'   | 1.90                     | 0.54              |
| 19:22:48:GLN:OE1  | 19:22:55:VAL:HG23 | 2.07                     | 0.54              |
| 21:24:20:LEU:HD11 | 21:24:27:PRO:HD3  | 1.89                     | 0.54              |
| 25:28:21:ALA:O    | 25:28:25:GLY:N    | 2.40                     | 0.54              |
| 30:33:38:LYS:HA   | 30:33:41:ARG:HE   | 1.72                     | 0.54              |
| 36:F:50:PRO:HD2   | 48:R:73:HIS:HB3   | 1.89                     | 0.54              |
| 38:H:21:LYS:O     | 38:H:62:LEU:HD12  | 2.07                     | 0.54              |
| 47:Q:3:LYS:HG2    | 47:Q:4:ILE:N      | 2.23                     | 0.54              |
| 47:Q:23:ALA:HA    | 47:Q:42:LYS:HA    | 1.90                     | 0.54              |
| 53:A:662:U:H2'    | 53:A:663:A:C8     | 2.42                     | 0.54              |
| 54:01:1827:U:O2'  | 54:01:1828:G:H5'  | 2.07                     | 0.54              |
| 2:05:142:VAL:HB   | 2:05:143:PRO:HD2  | 1.90                     | 0.54              |
| 3:06:52:VAL:HG13  | 54:01:452:G:OP1   | 2.07                     | 0.54              |
| 3:06:97:ASN:HB2   | 3:06:100:MET:SD   | 2.47                     | 0.54              |
| 3:06:192:ALA:O    | 3:06:196:VAL:HG23 | 2.07                     | 0.54              |
| 4:07:151:LEU:C    | 4:07:151:LEU:HD12 | 2.33                     | 0.54              |
| 7:10:3:LEU:CD1    | 7:10:6:GLN:H      | 2.17                     | 0.54              |
| 8:11:40:ALA:HB1   | 8:11:68:PHE:CE2   | 2.42                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:31:4:ILE:HG23  | 28:31:27:ARG:HD3  | 1.89                     | 0.54              |
| 36:F:29:ILE:HG21  | 36:F:64:VAL:HG21  | 1.89                     | 0.54              |
| 40:J:12:ALA:HB2   | 40:J:96:VAL:HG13  | 1.89                     | 0.54              |
| 47:Q:23:ALA:HB2   | 47:Q:42:LYS:HG2   | 1.89                     | 0.54              |
| 52:03:181:ASP:HB2 | 52:03:184:LYS:HG2 | 1.89                     | 0.54              |
| 54:01:741:U:H2'   | 54:01:742:A:C8    | 2.43                     | 0.54              |
| 54:01:1190:G:H2'  | 54:01:1191:G:H8   | 1.72                     | 0.54              |
| 10:13:26:GLY:O    | 10:13:30:ARG:HD2  | 2.07                     | 0.54              |
| 18:21:8:ARG:HB3   | 18:21:102:HIS:ND1 | 2.23                     | 0.54              |
| 27:30:54:ILE:HG23 | 27:30:56:LYS:H    | 1.73                     | 0.54              |
| 32:B:25:LYS:HD2   | 32:B:191:ASP:OD2  | 2.07                     | 0.54              |
| 34:D:62:ARG:HG3   | 34:D:62:ARG:HH11  | 1.73                     | 0.54              |
| 38:H:7:ALA:HB2    | 38:H:76:ARG:HG2   | 1.88                     | 0.54              |
| 39:I:46:VAL:HA    | 39:I:49:GLN:HG3   | 1.90                     | 0.54              |
| 43:M:96:VAL:N     | 53:A:1308:U:OP1   | 2.41                     | 0.54              |
| 43:M:100:ARG:HH12 | 53:A:950:U:H3'    | 1.73                     | 0.54              |
| 53:A:832:G:O2'    | 53:A:833:G:H5'    | 2.07                     | 0.54              |
| 54:01:196:A:H61   | 54:01:831:G:H21   | 1.56                     | 0.54              |
| 54:01:609:A:H2'   | 54:01:610:C:O4'   | 2.07                     | 0.54              |
| 54:01:713:G:H21   | 54:01:718:A:H62   | 1.56                     | 0.54              |
| 54:01:1386:C:H2'  | 54:01:1387:A:C8   | 2.43                     | 0.54              |
| 54:01:1956:U:H2'  | 54:01:1957:C:H5'  | 1.90                     | 0.54              |
| 54:01:2343:U:O2'  | 54:01:2344:U:H5'  | 2.08                     | 0.54              |
| 59:Z:4:SER:OG     | 59:Z:7:GLN:HB2    | 2.06                     | 0.54              |
| 6:09:73:ASN:HD21  | 6:09:76:GLU:HA    | 1.68                     | 0.54              |
| 7:10:87:GLU:OE2   | 7:10:95:LEU:HB2   | 2.08                     | 0.54              |
| 11:14:3:LEU:HD23  | 54:01:1203:U:H5'  | 1.90                     | 0.54              |
| 11:14:93:ASN:C    | 11:14:95:LEU:H    | 2.14                     | 0.54              |
| 17:20:89:HIS:HE1  | 17:20:91:GLN:HB2  | 1.73                     | 0.54              |
| 18:21:93:ALA:HB2  | 54:01:1614:A:C2   | 2.43                     | 0.54              |
| 25:28:37:ARG:HH21 | 54:01:929:U:H4'   | 1.73                     | 0.54              |
| 34:D:77:GLU:OE2   | 34:D:80:ARG:HD3   | 2.07                     | 0.54              |
| 37:G:149:ALA:HA   | 41:K:60:PHE:CD2   | 2.43                     | 0.54              |
| 39:I:116:GLY:C    | 39:I:117:LEU:HD12 | 2.33                     | 0.54              |
| 40:J:57:VAL:O     | 40:J:58:ASN:HB2   | 2.08                     | 0.54              |
| 42:L:74:GLN:C     | 42:L:76:HIS:H     | 2.14                     | 0.54              |
| 44:N:40:ARG:NH2   | 49:S:6:LYS:HD2    | 2.22                     | 0.54              |
| 49:S:30:LEU:H     | 49:S:48:ILE:HA    | 1.72                     | 0.54              |
| 51:U:38:GLU:HB2   | 53:A:1526:G:OP2   | 2.08                     | 0.54              |
| 54:01:511:U:H2'   | 54:01:512:G:H5'   | 1.89                     | 0.54              |
| 54:01:819:A:C2    | 54:01:820:A:C4    | 2.96                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:01:1669:A:O3'  | 54:01:2549:G:H5'  | 2.08                     | 0.54              |
| 54:01:2747:G:H21  | 54:01:2757:A:H62  | 1.56                     | 0.54              |
| 4:07:125:GLY:HA2  | 4:07:162:ASP:HA   | 1.90                     | 0.54              |
| 16:19:97:ILE:CD1  | 17:20:40:MET:HE1  | 2.38                     | 0.54              |
| 32:B:44:LYS:O     | 32:B:47:PRO:HG2   | 2.08                     | 0.54              |
| 32:B:72:LYS:CE    | 32:B:74:ALA:HB3   | 2.37                     | 0.54              |
| 37:G:111:GLY:HA2  | 37:G:118:ARG:CD   | 2.38                     | 0.54              |
| 39:I:121:ARG:HG3  | 53:A:1348:U:H4'   | 1.90                     | 0.54              |
| 40:J:22:THR:O     | 40:J:26:VAL:HG23  | 2.07                     | 0.54              |
| 43:M:26:LYS:O     | 43:M:30:LYS:HG3   | 2.08                     | 0.54              |
| 53:A:67:C:H2'     | 53:A:68:G:C8      | 2.43                     | 0.54              |
| 53:A:235:C:H2'    | 53:A:236:A:H8     | 1.73                     | 0.54              |
| 53:A:945:G:H2'    | 53:A:945:G:N3     | 2.23                     | 0.54              |
| 53:A:1137:C:H4'   | 53:A:1138:G:N2    | 2.23                     | 0.54              |
| 53:A:1502:A:H5'   | 53:A:1504:G:N7    | 2.23                     | 0.54              |
| 54:01:828:U:H2'   | 54:01:829:A:C8    | 2.42                     | 0.54              |
| 4:07:24:VAL:O     | 4:07:27:VAL:HG12  | 2.07                     | 0.54              |
| 4:07:118:ALA:HB1  | 4:07:166:ARG:HE   | 1.73                     | 0.54              |
| 18:21:60:HIS:CD2  | 54:01:486:C:H4'   | 2.43                     | 0.54              |
| 27:30:43:THR:HG23 | 27:30:47:TYR:O    | 2.08                     | 0.54              |
| 37:G:12:LEU:HD11  | 39:I:49:GLN:NE2   | 2.13                     | 0.54              |
| 37:G:71:THR:HA    | 37:G:95:ARG:NH1   | 2.22                     | 0.54              |
| 41:K:93:GLU:O     | 41:K:96:ILE:HG12  | 2.07                     | 0.54              |
| 43:M:16:ILE:HD12  | 43:M:16:ILE:N     | 2.23                     | 0.54              |
| 47:Q:29:LYS:HB2   | 47:Q:36:PHE:CE1   | 2.43                     | 0.54              |
| 54:01:776:G:H22   | 54:01:2072:C:H5'  | 1.73                     | 0.54              |
| 7:10:118:ILE:HG22 | 7:10:118:ILE:O    | 2.07                     | 0.53              |
| 8:11:7:TYR:C      | 8:11:7:TYR:CD1    | 2.86                     | 0.53              |
| 16:19:75:TYR:O    | 16:19:78:PHE:HB3  | 2.08                     | 0.53              |
| 18:21:3:THR:HG21  | 18:21:58:ALA:HA   | 1.90                     | 0.53              |
| 18:21:97:LEU:HD12 | 18:21:97:LEU:N    | 2.24                     | 0.53              |
| 35:E:67:ARG:O     | 35:E:70:MET:HG3   | 2.08                     | 0.53              |
| 39:I:56:MET:O     | 39:I:57:VAL:C     | 2.50                     | 0.53              |
| 47:Q:57:VAL:HG12  | 47:Q:58:VAL:N     | 2.23                     | 0.53              |
| 52:03:50:ILE:HG22 | 52:03:204:ALA:HB1 | 1.90                     | 0.53              |
| 53:A:79:G:O2'     | 53:A:80:A:H5'     | 2.08                     | 0.53              |
| 53:A:352:C:H4'    | 53:A:354:G:OP1    | 2.07                     | 0.53              |
| 54:01:2737:G:H2'  | 54:01:2738:A:C8   | 2.43                     | 0.53              |
| 55:02:30:C:H2'    | 55:02:31:C:O4'    | 2.08                     | 0.53              |
| 56:X:68:C:H2'     | 56:X:69:C:O4'     | 2.07                     | 0.53              |
| 3:06:63:LYS:NZ    | 54:01:2060:A:H3'  | 2.22                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:15:3:GLN:HE21  | 12:15:92:TRP:HE1  | 1.56                     | 0.53              |
| 23:26:63:ILE:O    | 23:26:67:LEU:HD13 | 2.09                     | 0.53              |
| 26:29:12:ILE:HD13 | 26:29:26:SER:HB3  | 1.90                     | 0.53              |
| 36:F:38:ARG:HH21  | 36:F:100:SER:HB2  | 1.72                     | 0.53              |
| 43:M:15:VAL:CG2   | 43:M:16:ILE:HD12  | 2.31                     | 0.53              |
| 53:A:225:C:H3'    | 53:A:226:G:H5''   | 1.90                     | 0.53              |
| 53:A:1273:C:H2'   | 53:A:1274:A:O4'   | 2.09                     | 0.53              |
| 53:A:1346:A:H2'   | 53:A:1346:A:N3    | 2.23                     | 0.53              |
| 54:01:1053:C:H3'  | 54:01:1054:A:H5'' | 1.90                     | 0.53              |
| 55:02:114:C:H2'   | 55:02:115:A:C8    | 2.42                     | 0.53              |
| 2:05:51:THR:HB    | 2:05:79:LEU:HD23  | 1.89                     | 0.53              |
| 2:05:149:ASN:HB3  | 54:01:2572:A:OP2  | 2.08                     | 0.53              |
| 5:08:21:GLN:NE2   | 5:08:36:LEU:HB2   | 2.19                     | 0.53              |
| 16:19:90:ASP:OD2  | 16:19:92:LYS:HB3  | 2.08                     | 0.53              |
| 36:F:4:TYR:O      | 36:F:63:ASN:HA    | 2.09                     | 0.53              |
| 42:L:21:PRO:HD2   | 42:L:93:ARG:HH21  | 1.73                     | 0.53              |
| 49:S:2:ARG:O      | 49:S:3:SER:HB3    | 2.07                     | 0.53              |
| 53:A:880:C:H2'    | 53:A:881:G:H8     | 1.72                     | 0.53              |
| 54:01:466:A:C2'   | 54:01:467:G:H5'   | 2.38                     | 0.53              |
| 4:07:70:ARG:HG2   | 4:07:70:ARG:HH21  | 1.74                     | 0.53              |
| 5:08:68:ARG:HG2   | 5:08:68:ARG:HH11  | 1.74                     | 0.53              |
| 13:16:2:ARG:HA    | 13:16:5:LYS:CD    | 2.38                     | 0.53              |
| 34:D:56:GLU:O     | 34:D:60:VAL:HG23  | 2.08                     | 0.53              |
| 35:E:80:LEU:HD21  | 35:E:95:MET:SD    | 2.49                     | 0.53              |
| 35:E:110:MET:HG3  | 35:E:139:THR:HG21 | 1.90                     | 0.53              |
| 36:F:90:MET:SD    | 48:R:22:TYR:HE2   | 2.30                     | 0.53              |
| 40:J:15:HIS:C     | 40:J:17:LEU:H     | 2.17                     | 0.53              |
| 40:J:101:SER:C    | 40:J:102:LEU:HD12 | 2.33                     | 0.53              |
| 41:K:15:VAL:HG22  | 41:K:16:SER:N     | 2.22                     | 0.53              |
| 46:P:48:GLU:HG3   | 46:P:49:GLY:N     | 2.18                     | 0.53              |
| 53:A:1219:A:H2'   | 53:A:1220:G:C8    | 2.44                     | 0.53              |
| 54:01:542:C:H2'   | 54:01:543:G:H5''  | 1.90                     | 0.53              |
| 16:19:24:TYR:HE1  | 54:01:17:G:H4'    | 1.73                     | 0.53              |
| 17:20:78:ARG:HB2  | 17:20:83:TYR:HD2  | 1.74                     | 0.53              |
| 18:21:24:ILE:HD11 | 18:21:74:ILE:CD1  | 2.39                     | 0.53              |
| 37:G:15:PRO:HG2   | 37:G:43:TYR:OH    | 2.07                     | 0.53              |
| 42:L:29:LYS:O     | 42:L:80:LEU:HD12  | 2.08                     | 0.53              |
| 44:N:92:ILE:H     | 44:N:92:ILE:CD1   | 2.15                     | 0.53              |
| 53:A:736:C:H2'    | 53:A:737:C:C6     | 2.43                     | 0.53              |
| 54:01:2078:C:H2'  | 54:01:2079:U:C6   | 2.44                     | 0.53              |
| 54:01:2404:U:H2'  | 54:01:2405:G:O4'  | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 56:X:25:C:N4      | 56:X:45:G:H22     | 2.07                     | 0.53              |
| 4:07:3:LEU:HG     | 4:07:100:GLU:OE1  | 2.08                     | 0.53              |
| 7:10:57:ASN:O     | 7:10:59:LEU:N     | 2.41                     | 0.53              |
| 21:24:27:PRO:O    | 21:24:88:HIS:HA   | 2.09                     | 0.53              |
| 32:B:16:GLY:CA    | 59:Z:43:LYS:HD2   | 2.39                     | 0.53              |
| 33:C:116:ALA:HB1  | 33:C:186:SER:OG   | 2.08                     | 0.53              |
| 34:D:85:THR:HB    | 35:E:102:THR:HG21 | 1.90                     | 0.53              |
| 35:E:159:SER:HB3  | 35:E:162:GLU:HG2  | 1.90                     | 0.53              |
| 35:E:163:ILE:HD12 | 35:E:163:ILE:C    | 2.34                     | 0.53              |
| 54:01:1038:G:H2'  | 54:01:1039:A:C8   | 2.44                     | 0.53              |
| 54:01:2036:C:H2'  | 54:01:2037:A:C8   | 2.43                     | 0.53              |
| 54:01:2487:G:H2'  | 54:01:2488:G:C8   | 2.43                     | 0.53              |
| 54:01:2834:G:H2'  | 54:01:2879:A:H61  | 1.74                     | 0.53              |
| 3:06:149:ILE:CG2  | 3:06:188:MET:HG2  | 2.37                     | 0.53              |
| 8:11:34:ILE:H     | 8:11:34:ILE:CD1   | 2.21                     | 0.53              |
| 10:13:63:VAL:HG23 | 10:13:64:ARG:H    | 1.72                     | 0.53              |
| 13:16:82:GLU:O    | 13:16:85:PRO:HG2  | 2.09                     | 0.53              |
| 16:19:49:ARG:CZ   | 17:20:72:VAL:HG13 | 2.39                     | 0.53              |
| 16:19:111:LYS:HG2 | 17:20:48:LYS:HD2  | 1.90                     | 0.53              |
| 22:25:42:HIS:HB2  | 22:25:75:PHE:CE1  | 2.43                     | 0.53              |
| 32:B:16:GLY:C     | 59:Z:43:LYS:HD2   | 2.34                     | 0.53              |
| 40:J:98:VAL:HG22  | 40:J:99:GLN:N     | 2.24                     | 0.53              |
| 50:T:70:LYS:HA    | 50:T:73:ARG:HH12  | 1.74                     | 0.53              |
| 53:A:229:U:H2'    | 53:A:230:G:C8     | 2.43                     | 0.53              |
| 54:01:833:A:H2'   | 54:01:834:G:C8    | 2.43                     | 0.53              |
| 9:12:27:ARG:HH11  | 9:12:27:ARG:HG3   | 1.74                     | 0.53              |
| 9:12:99:ARG:HD2   | 9:12:102:GLU:OE1  | 2.09                     | 0.53              |
| 10:13:76:VAL:HG12 | 15:18:72:VAL:HG22 | 1.90                     | 0.53              |
| 13:16:2:ARG:HA    | 13:16:5:LYS:HE2   | 1.91                     | 0.53              |
| 34:D:195:ASN:HD22 | 34:D:198:LEU:CG   | 2.17                     | 0.53              |
| 35:E:39:GLY:HA3   | 35:E:45:VAL:HG12  | 1.91                     | 0.53              |
| 48:R:11:ARG:HH21  | 48:R:11:ARG:HG2   | 1.73                     | 0.53              |
| 53:A:82:G:H2'     | 53:A:83:C:O4'     | 2.09                     | 0.53              |
| 53:A:1004:A:H2'   | 53:A:1005:A:O4'   | 2.08                     | 0.53              |
| 54:01:765:C:H2'   | 54:01:766:U:C6    | 2.43                     | 0.53              |
| 54:01:1196:C:H2'  | 54:01:1197:G:H8   | 1.72                     | 0.53              |
| 54:01:1657:U:H2'  | 54:01:1658:C:H6   | 1.74                     | 0.53              |
| 54:01:2743:U:C2'  | 54:01:2744:G:H5'' | 2.38                     | 0.53              |
| 55:02:35:C:H2'    | 55:02:36:C:H5'    | 1.89                     | 0.53              |
| 3:06:29:HIS:O     | 3:06:32:VAL:HG12  | 2.08                     | 0.53              |
| 6:09:51:ARG:HG2   | 6:09:55:GLU:OE1   | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:16:103:ARG:NH1 | 54:01:1287:A:H5'  | 2.24                     | 0.53              |
| 16:19:24:TYR:O    | 16:19:27:ARG:HB2  | 2.09                     | 0.53              |
| 17:20:6:GLN:HA    | 17:20:10:LYS:O    | 2.08                     | 0.53              |
| 32:B:96:LEU:HB2   | 32:B:99:MET:HG3   | 1.90                     | 0.53              |
| 34:D:119:HIS:ND1  | 53:A:438:U:H4'    | 2.24                     | 0.53              |
| 43:M:2:ARG:NE     | 43:M:8:ILE:HD11   | 2.11                     | 0.53              |
| 43:M:22:TYR:CE1   | 53:A:1330:U:H4'   | 2.44                     | 0.53              |
| 53:A:1326:U:O2'   | 53:A:1327:C:H5'   | 2.08                     | 0.53              |
| 54:01:11:C:H2'    | 54:01:12:U:H5''   | 1.91                     | 0.53              |
| 57:V:17:U:O2'     | 57:V:18:G:H5'     | 2.07                     | 0.53              |
| 3:06:19:PHE:HE1   | 3:06:109:LEU:HD23 | 1.74                     | 0.53              |
| 8:11:35:MET:O     | 8:11:39:LYS:HG2   | 2.09                     | 0.53              |
| 17:20:37:GLU:O    | 17:20:38:VAL:C    | 2.52                     | 0.53              |
| 20:23:50:ALA:C    | 20:23:52:ASN:H    | 2.17                     | 0.53              |
| 21:24:65:VAL:HG13 | 21:24:65:VAL:O    | 2.08                     | 0.53              |
| 33:C:141:MET:HE2  | 33:C:169:GLU:HG3  | 1.90                     | 0.53              |
| 34:D:170:LEU:HD12 | 34:D:170:LEU:C    | 2.34                     | 0.53              |
| 35:E:106:ALA:HB2  | 35:E:124:ALA:HB3  | 1.91                     | 0.53              |
| 39:I:94:ARG:O     | 39:I:98:ARG:N     | 2.42                     | 0.53              |
| 41:K:21:HIS:NE2   | 41:K:84:MET:HE3   | 2.23                     | 0.53              |
| 46:P:29:ASN:ND2   | 46:P:29:ASN:N     | 2.56                     | 0.53              |
| 47:Q:4:ILE:HD12   | 47:Q:4:ILE:O      | 2.08                     | 0.53              |
| 53:A:166:U:H2'    | 53:A:167:A:C8     | 2.44                     | 0.53              |
| 53:A:626:G:H2'    | 53:A:627:G:H8     | 1.74                     | 0.53              |
| 53:A:1464:U:H2'   | 53:A:1465:A:C8    | 2.44                     | 0.53              |
| 54:01:84:A:H4'    | 54:01:85:G:O5'    | 2.09                     | 0.53              |
| 54:01:115:C:O2'   | 54:01:116:C:H5'   | 2.09                     | 0.53              |
| 54:01:546:U:H2'   | 54:01:547:A:C4'   | 2.40                     | 0.53              |
| 54:01:1979:U:H2'  | 54:01:1980:G:C8   | 2.43                     | 0.53              |
| 54:01:2629:U:O2'  | 54:01:2630:G:H5'' | 2.08                     | 0.53              |
| 3:06:73:ILE:O     | 3:06:73:ILE:HG12  | 2.08                     | 0.52              |
| 3:06:196:VAL:O    | 3:06:200:LEU:HD13 | 2.09                     | 0.52              |
| 19:22:5:GLU:HA    | 19:22:8:LEU:HD12  | 1.89                     | 0.52              |
| 33:C:108:PRO:HA   | 33:C:114:LEU:CD1  | 2.39                     | 0.52              |
| 35:E:106:ALA:CB   | 35:E:124:ALA:HB3  | 2.39                     | 0.52              |
| 41:K:41:LEU:HD13  | 41:K:78:ILE:HD11  | 1.91                     | 0.52              |
| 42:L:33:CYS:HB2   | 42:L:79:ILE:HG13  | 1.90                     | 0.52              |
| 54:01:760:G:H2'   | 54:01:761:A:O4'   | 2.08                     | 0.52              |
| 59:Z:12:SER:HA    | 59:Z:15:GLU:OE1   | 2.09                     | 0.52              |
| 2:05:121:THR:HB   | 2:05:127:PHE:CD2  | 2.44                     | 0.52              |
| 2:05:136:ASN:HA   | 54:01:2579:C:O2'  | 2.09                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:09:4:ILE:H       | 6:09:39:ALA:HB2   | 1.74                     | 0.52              |
| 12:15:132:THR:HG22 | 12:15:133:LYS:N   | 2.24                     | 0.52              |
| 42:L:35:ARG:HG2    | 42:L:37:TYR:CD2   | 2.44                     | 0.52              |
| 42:L:43:LYS:HB3    | 42:L:44:PRO:HD3   | 1.91                     | 0.52              |
| 43:M:106:ARG:HE    | 43:M:112:ARG:HH21 | 1.57                     | 0.52              |
| 45:O:7:THR:O       | 45:O:11:VAL:HG23  | 2.09                     | 0.52              |
| 46:P:46:LYS:HZ2    | 46:P:48:GLU:HB3   | 1.75                     | 0.52              |
| 53:A:883:C:O2'     | 53:A:884:U:H5'    | 2.09                     | 0.52              |
| 54:01:1297:C:OP1   | 54:01:2710:C:H4'  | 2.09                     | 0.52              |
| 54:01:1437:C:H2'   | 54:01:1438:U:C6   | 2.44                     | 0.52              |
| 54:01:2208:C:H2'   | 54:01:2209:G:C8   | 2.44                     | 0.52              |
| 2:05:89:GLU:HG3    | 2:05:90:PHE:N     | 2.24                     | 0.52              |
| 18:21:25:ARG:NH2   | 54:01:519:U:H5''  | 2.24                     | 0.52              |
| 38:H:45:ILE:HD13   | 38:H:60:LEU:HD13  | 1.90                     | 0.52              |
| 38:H:72:GLU:HB3    | 38:H:129:ALA:C    | 2.34                     | 0.52              |
| 38:H:95:MET:C      | 38:H:97:GLY:N     | 2.67                     | 0.52              |
| 50:T:8:LYS:O       | 50:T:11:ILE:HG12  | 2.09                     | 0.52              |
| 50:T:57:VAL:HG13   | 50:T:58:ASP:N     | 2.24                     | 0.52              |
| 53:A:312:C:H2'     | 53:A:313:A:H8     | 1.74                     | 0.52              |
| 1:04:7:PRO:HB3     | 1:04:13:ARG:HA    | 1.92                     | 0.52              |
| 1:04:196:ASN:ND2   | 1:04:199:HIS:HB2  | 2.24                     | 0.52              |
| 3:06:137:LYS:HA    | 3:06:140:ASP:OD2  | 2.09                     | 0.52              |
| 5:08:136:ASP:OD2   | 5:08:139:VAL:HG23 | 2.09                     | 0.52              |
| 7:10:120:ALA:O     | 7:10:121:SER:HB2  | 2.09                     | 0.52              |
| 10:13:2:ILE:HG23   | 10:13:6:THR:HG21  | 1.92                     | 0.52              |
| 26:29:11:GLU:HA    | 26:29:25:ARG:HG2  | 1.90                     | 0.52              |
| 34:D:79:ALA:HA     | 34:D:85:THR:HG23  | 1.92                     | 0.52              |
| 39:I:64:ILE:HD13   | 39:I:78:ILE:HG23  | 1.92                     | 0.52              |
| 53:A:77:A:H2'      | 53:A:78:A:C8      | 2.45                     | 0.52              |
| 54:01:141:G:H3'    | 54:01:142:A:O4'   | 2.09                     | 0.52              |
| 54:01:167:A:H2'    | 54:01:168:G:O4'   | 2.10                     | 0.52              |
| 54:01:474:G:O2'    | 54:01:475:C:H5''  | 2.09                     | 0.52              |
| 54:01:1367:A:C2'   | 54:01:1368:G:H5'  | 2.40                     | 0.52              |
| 54:01:2277:G:C3'   | 54:01:2278:A:H5'' | 2.39                     | 0.52              |
| 54:01:2391:G:H4'   | 54:01:2392:A:OP1  | 2.08                     | 0.52              |
| 54:01:2515:C:H2'   | 54:01:2516:A:C8   | 2.43                     | 0.52              |
| 54:01:2698:U:H2'   | 54:01:2699:C:C6   | 2.44                     | 0.52              |
| 5:08:2:ARG:HD2     | 54:01:2751:G:OP2  | 2.09                     | 0.52              |
| 5:08:4:ALA:HB2     | 5:08:65:GLY:HA2   | 1.92                     | 0.52              |
| 5:08:43:LYS:HB2    | 5:08:50:THR:OG1   | 2.08                     | 0.52              |
| 16:19:56:PHE:CZ    | 54:01:536:G:H4'   | 2.43                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:D:36:ALA:N     | 34:D:37:PRO:CD     | 2.73                     | 0.52              |
| 35:E:105:ILE:HA   | 35:E:111:ARG:HH22  | 1.73                     | 0.52              |
| 36:F:79:ARG:HG2   | 36:F:79:ARG:HH11   | 1.74                     | 0.52              |
| 39:I:17:ARG:HH12  | 53:A:1129:C:H4'    | 1.75                     | 0.52              |
| 52:O3:46:VAL:O    | 52:O3:171:ILE:HG22 | 2.09                     | 0.52              |
| 53:A:952:U:H2'    | 53:A:953:G:C8      | 2.45                     | 0.52              |
| 54:O1:1298:C:H2'  | 54:O1:1299:G:O4'   | 2.10                     | 0.52              |
| 54:O1:1424:G:H2'  | 54:O1:1425:G:O4'   | 2.09                     | 0.52              |
| 54:O1:1527:G:H21  | 54:O1:1545:A:H62   | 1.58                     | 0.52              |
| 56:W:20:U:H3'     | 56:W:21:A:H5'      | 1.90                     | 0.52              |
| 1:O4:87:SER:O     | 1:O4:157:ALA:HB2   | 2.10                     | 0.52              |
| 4:O7:54:ALA:O     | 4:O7:57:ALA:HB3    | 2.10                     | 0.52              |
| 7:10:47:GLU:CD    | 7:10:95:LEU:HD11   | 2.35                     | 0.52              |
| 11:14:86:GLU:O    | 11:14:89:VAL:HG12  | 2.10                     | 0.52              |
| 12:15:11:LYS:HD3  | 12:15:86:LYS:HG2   | 1.92                     | 0.52              |
| 32:B:113:LEU:O    | 32:B:117:GLU:HG3   | 2.09                     | 0.52              |
| 35:E:160:VAL:HG13 | 35:E:161:GLU:N     | 2.24                     | 0.52              |
| 37:G:71:THR:HG23  | 37:G:95:ARG:HH12   | 1.73                     | 0.52              |
| 38:H:5:PRO:O      | 38:H:32:LYS:HE2    | 2.10                     | 0.52              |
| 47:Q:13:SER:HB3   | 47:Q:21:VAL:HG11   | 1.91                     | 0.52              |
| 51:U:58:LYS:O     | 51:U:61:ARG:HG2    | 2.09                     | 0.52              |
| 53:A:1254:A:H2'   | 53:A:1255:G:C8     | 2.45                     | 0.52              |
| 54:O1:832:U:H2'   | 54:O1:833:A:C8     | 2.45                     | 0.52              |
| 54:O1:1045:C:OP1  | 54:O1:1047:G:H5'   | 2.10                     | 0.52              |
| 54:O1:2730:C:H2'  | 54:O1:2731:G:C8    | 2.45                     | 0.52              |
| 1:O4:250:GLN:O    | 1:O4:254:LYS:HB3   | 2.09                     | 0.52              |
| 2:O5:30:GLU:O     | 2:O5:31:ALA:C      | 2.53                     | 0.52              |
| 7:10:88:HIS:N     | 7:10:89:PRO:HD2    | 2.24                     | 0.52              |
| 8:11:21:PRO:CB    | 8:11:22:PRO:HD3    | 2.40                     | 0.52              |
| 43:M:28:ARG:NH2   | 43:M:62:PHE:HB2    | 2.24                     | 0.52              |
| 53:A:77:A:H2'     | 53:A:78:A:H8       | 1.75                     | 0.52              |
| 53:A:513:C:H2'    | 53:A:514:C:C6      | 2.45                     | 0.52              |
| 53:A:1219:A:H2'   | 53:A:1220:G:H8     | 1.74                     | 0.52              |
| 54:O1:885:C:N4    | 54:O1:886:A:H62    | 2.07                     | 0.52              |
| 54:O1:1386:C:H2'  | 54:O1:1387:A:H8    | 1.74                     | 0.52              |
| 54:O1:1417:C:H4'  | 54:O1:1587:G:H21   | 1.73                     | 0.52              |
| 54:O1:1810:A:H2'  | 54:O1:1811:G:O4'   | 2.10                     | 0.52              |
| 54:O1:2475:C:H2'  | 54:O1:2476:A:H5'   | 1.92                     | 0.52              |
| 54:O1:2737:G:H2'  | 54:O1:2738:A:H8    | 1.73                     | 0.52              |
| 54:O1:2837:A:H2'  | 54:O1:2838:G:C8    | 2.44                     | 0.52              |
| 59:Z:150:LYS:HG2  | 59:Z:152:LEU:HD23  | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:09:96:THR:HG22  | 6:09:117:LEU:HD12 | 1.90                     | 0.52              |
| 8:11:15:GLY:O     | 8:11:16:MET:HE2   | 2.10                     | 0.52              |
| 17:20:15:SER:O    | 17:20:18:GLN:HG2  | 2.10                     | 0.52              |
| 19:22:67:VAL:HG22 | 19:22:76:ARG:HG3  | 1.90                     | 0.52              |
| 22:25:45:ALA:O    | 22:25:47:VAL:HG23 | 2.09                     | 0.52              |
| 32:B:166:ASP:OD2  | 32:B:190:SER:HA   | 2.10                     | 0.52              |
| 41:K:80:ASN:HA    | 41:K:105:ARG:HB2  | 1.92                     | 0.52              |
| 43:M:94:LEU:HB3   | 43:M:95:PRO:HD2   | 1.92                     | 0.52              |
| 46:P:18:GLN:HE21  | 46:P:35:ARG:HH21  | 1.58                     | 0.52              |
| 53:A:434:U:H2'    | 53:A:435:A:H8     | 1.73                     | 0.52              |
| 53:A:673:A:H2'    | 53:A:674:G:C8     | 2.44                     | 0.52              |
| 54:01:680:C:H2'   | 54:01:681:G:C8    | 2.45                     | 0.52              |
| 54:01:1176:U:H2'  | 54:01:1177:G:C8   | 2.45                     | 0.52              |
| 54:01:1278:C:H2'  | 54:01:1279:G:C8   | 2.45                     | 0.52              |
| 54:01:1357:C:H2'  | 54:01:1358:G:O4'  | 2.10                     | 0.52              |
| 3:06:88:ARG:O     | 3:06:90:GLN:N     | 2.42                     | 0.52              |
| 5:08:155:PRO:HG3  | 54:01:2530:A:N6   | 2.25                     | 0.52              |
| 6:09:9:VAL:HB     | 6:09:13:GLY:HA3   | 1.91                     | 0.52              |
| 9:12:114:LEU:HG   | 9:12:118:MET:HE3  | 1.92                     | 0.52              |
| 22:25:22:PHE:HD2  | 54:01:922:C:H1'   | 1.75                     | 0.52              |
| 28:31:36:LYS:HG2  | 28:31:45:HIS:HB3  | 1.91                     | 0.52              |
| 34:D:166:LYS:N    | 34:D:167:PRO:HD3  | 2.25                     | 0.52              |
| 51:U:11:PHE:CD1   | 51:U:12:ASP:N     | 2.78                     | 0.52              |
| 51:U:36:PHE:HB3   | 51:U:40:PRO:CD    | 2.39                     | 0.52              |
| 53:A:422:C:H5'    | 53:A:423:G:C4     | 2.45                     | 0.52              |
| 53:A:1238:A:H2'   | 53:A:1239:A:H5'   | 1.91                     | 0.52              |
| 54:01:1278:C:H2'  | 54:01:1279:G:H8   | 1.73                     | 0.52              |
| 54:01:1285:A:H2'  | 54:01:1286:A:H5'  | 1.92                     | 0.52              |
| 54:01:1539:U:H2'  | 54:01:1540:G:C8   | 2.42                     | 0.52              |
| 54:01:2293:G:H2'  | 54:01:2294:G:C8   | 2.45                     | 0.52              |
| 1:04:175:LEU:HB2  | 1:04:179:GLU:HB3  | 1.92                     | 0.52              |
| 3:06:143:LEU:HB3  | 3:06:146:VAL:HG11 | 1.92                     | 0.52              |
| 5:08:174:LYS:HG2  | 5:08:175:LYS:N    | 2.25                     | 0.52              |
| 8:11:7:TYR:HA     | 8:11:58:ILE:O     | 2.09                     | 0.52              |
| 14:17:31:THR:HG22 | 14:17:33:ARG:H    | 1.75                     | 0.52              |
| 25:28:12:ALA:HB2  | 25:28:23:LEU:HD12 | 1.91                     | 0.52              |
| 25:28:17:PRO:HG2  | 54:01:968:C:H5''  | 1.91                     | 0.52              |
| 31:34:4:ARG:HB3   | 54:01:2466:C:OP1  | 2.10                     | 0.52              |
| 43:M:52:ILE:O     | 43:M:55:LEU:HB3   | 2.10                     | 0.52              |
| 46:P:44:SER:C     | 46:P:46:LYS:H     | 2.18                     | 0.52              |
| 53:A:423:G:H2'    | 53:A:424:G:H5'    | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:A:916:U:H2'    | 53:A:917:G:H8     | 1.74                     | 0.52              |
| 54:01:598:U:H2'   | 54:01:599:A:C8    | 2.45                     | 0.52              |
| 54:01:1062:G:OP1  | 54:01:1070:A:H5'' | 2.10                     | 0.52              |
| 3:06:197:GLU:O    | 3:06:201:ALA:N    | 2.37                     | 0.51              |
| 4:07:102:LEU:O    | 4:07:107:VAL:HG23 | 2.10                     | 0.51              |
| 7:10:40:GLU:O     | 7:10:43:LYS:HB3   | 2.10                     | 0.51              |
| 20:23:66:VAL:O    | 20:23:69:VAL:HG22 | 2.10                     | 0.51              |
| 36:F:61:LEU:HD12  | 36:F:62:MET:H     | 1.74                     | 0.51              |
| 41:K:88:PRO:HD3   | 51:U:28:LEU:HD11  | 1.92                     | 0.51              |
| 47:Q:63:CYS:SG    | 47:Q:73:THR:N     | 2.84                     | 0.51              |
| 49:S:69:LYS:HE3   | 53:A:1319:A:H5''  | 1.93                     | 0.51              |
| 50:T:67:HIS:ND1   | 50:T:67:HIS:O     | 2.43                     | 0.51              |
| 53:A:16:A:O2'     | 53:A:17:U:H5'     | 2.09                     | 0.51              |
| 54:01:145:C:H2'   | 54:01:146:A:C8    | 2.45                     | 0.51              |
| 54:01:1790:C:H2'  | 54:01:1791:A:C5   | 2.45                     | 0.51              |
| 54:01:2358:A:H2'  | 54:01:2359:C:O4'  | 2.10                     | 0.51              |
| 54:01:2591:C:H2'  | 54:01:2592:G:C8   | 2.45                     | 0.51              |
| 5:08:98:LYS:NZ    | 5:08:103:ASN:HD22 | 2.09                     | 0.51              |
| 6:09:29:PHE:O     | 6:09:32:PRO:HG2   | 2.09                     | 0.51              |
| 11:14:101:ILE:CG1 | 11:14:102:GLY:H   | 2.14                     | 0.51              |
| 13:16:99:LYS:O    | 27:30:41:HIS:HA   | 2.09                     | 0.51              |
| 17:20:14:VAL:HG22 | 17:20:15:SER:N    | 2.25                     | 0.51              |
| 17:20:14:VAL:HG21 | 17:20:98:ILE:HG13 | 1.90                     | 0.51              |
| 26:29:58:ASP:HA   | 26:29:61:ASN:HD22 | 1.72                     | 0.51              |
| 27:30:54:ILE:HG23 | 27:30:55:ALA:N    | 2.24                     | 0.51              |
| 54:01:1856:U:H2'  | 54:01:1857:G:O4'  | 2.10                     | 0.51              |
| 54:01:2104:C:H2'  | 54:01:2105:U:C6   | 2.45                     | 0.51              |
| 55:02:30:C:C2'    | 55:02:31:C:H5'    | 2.40                     | 0.51              |
| 3:06:5:LEU:HD13   | 3:06:10:SER:O     | 2.10                     | 0.51              |
| 4:07:142:TYR:O    | 4:07:145:VAL:HG22 | 2.11                     | 0.51              |
| 8:11:99:LYS:HA    | 8:11:138:VAL:O    | 2.10                     | 0.51              |
| 12:15:59:ARG:HG3  | 12:15:59:ARG:HH21 | 1.73                     | 0.51              |
| 16:19:55:GLN:HE21 | 54:01:559:G:H1'   | 1.74                     | 0.51              |
| 22:25:7:ARG:HG2   | 22:25:7:ARG:HH11  | 1.75                     | 0.51              |
| 26:29:16:CYS:SG   | 26:29:20:ASN:HB3  | 2.50                     | 0.51              |
| 31:34:25:VAL:HB   | 31:34:35:GLN:CG   | 2.40                     | 0.51              |
| 34:D:68:GLU:HB3   | 53:A:546:A:P      | 2.50                     | 0.51              |
| 34:D:169:TRP:HE1  | 34:D:170:LEU:HD23 | 1.75                     | 0.51              |
| 35:E:155:LYS:HG3  | 35:E:156:ARG:HG2  | 1.93                     | 0.51              |
| 36:F:92:THR:OG1   | 36:F:93:LYS:N     | 2.43                     | 0.51              |
| 37:G:119:LEU:C    | 37:G:119:LEU:HD23 | 2.36                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:L:35:ARG:HG2   | 42:L:37:TYR:HD2    | 1.74                     | 0.51              |
| 53:A:1200:C:H5''  | 53:A:1201:A:H3'    | 1.92                     | 0.51              |
| 54:01:596:U:H2'   | 54:01:597:G:H8     | 1.73                     | 0.51              |
| 54:01:1786:A:H1'  | 54:01:1938:A:N6    | 2.25                     | 0.51              |
| 54:01:2163:A:H2'  | 54:01:2164:C:H5'   | 1.91                     | 0.51              |
| 54:01:2360:G:H2'  | 54:01:2361:G:H5'   | 1.93                     | 0.51              |
| 58:Y:25:C:H2'     | 58:Y:26:A:H8       | 1.76                     | 0.51              |
| 2:05:148:GLN:HB2  | 2:05:152:PRO:HG2   | 1.91                     | 0.51              |
| 4:07:4:HIS:CD2    | 4:07:8:LYS:HE3     | 2.46                     | 0.51              |
| 12:15:35:ALA:HA   | 12:15:128:THR:HG22 | 1.93                     | 0.51              |
| 18:21:40:ASN:O    | 18:21:41:LYS:HG2   | 2.09                     | 0.51              |
| 27:30:49:ARG:HG2  | 54:01:2884:U:C6    | 2.45                     | 0.51              |
| 45:O:87:ARG:O     | 45:O:87:ARG:HG3    | 2.09                     | 0.51              |
| 51:U:29:ALA:HA    | 51:U:32:ARG:HD3    | 1.92                     | 0.51              |
| 53:A:312:C:H2'    | 53:A:313:A:C8      | 2.46                     | 0.51              |
| 53:A:361:G:H2'    | 53:A:362:G:O4'     | 2.10                     | 0.51              |
| 53:A:731:G:O2'    | 53:A:732:C:H5'     | 2.11                     | 0.51              |
| 53:A:990:C:H2'    | 53:A:991:U:O4'     | 2.09                     | 0.51              |
| 54:01:250:G:N1    | 54:01:251:A:C2     | 2.79                     | 0.51              |
| 54:01:1289:C:H2'  | 54:01:1290:C:H6    | 1.75                     | 0.51              |
| 1:04:1:ALA:N      | 1:04:19:VAL:O      | 2.43                     | 0.51              |
| 1:04:224:MET:HG2  | 54:01:782:A:N3     | 2.25                     | 0.51              |
| 17:20:58:VAL:O    | 17:20:102:SER:HB2  | 2.11                     | 0.51              |
| 18:21:1:MET:N     | 18:21:110:ARG:HH11 | 2.09                     | 0.51              |
| 32:B:166:ASP:CG   | 32:B:190:SER:HA    | 2.36                     | 0.51              |
| 47:Q:46:HIS:CA    | 47:Q:70:LYS:HD2    | 2.40                     | 0.51              |
| 53:A:212:G:H2'    | 53:A:213:G:H8      | 1.76                     | 0.51              |
| 53:A:477:C:H2'    | 53:A:478:A:C8      | 2.46                     | 0.51              |
| 53:A:543:U:H2'    | 53:A:544:G:C8      | 2.45                     | 0.51              |
| 53:A:985:C:H2'    | 53:A:986:U:C6      | 2.46                     | 0.51              |
| 53:A:1071:C:H2'   | 53:A:1072:G:H8     | 1.76                     | 0.51              |
| 53:A:1170:A:H2'   | 53:A:1171:A:O4'    | 2.10                     | 0.51              |
| 54:01:833:A:H2'   | 54:01:834:G:H8     | 1.75                     | 0.51              |
| 54:01:1506:U:H2'  | 54:01:1507:C:C6    | 2.45                     | 0.51              |
| 54:01:2843:G:O2'  | 54:01:2844:G:H5'   | 2.11                     | 0.51              |
| 1:04:62:ARG:HG3   | 1:04:62:ARG:NH1    | 2.26                     | 0.51              |
| 33:C:113:LYS:N    | 33:C:184:ASN:ND2   | 2.59                     | 0.51              |
| 35:E:113:VAL:HG13 | 35:E:114:LEU:CD1   | 2.40                     | 0.51              |
| 42:L:2:THR:HG22   | 42:L:5:GLN:HG3     | 1.92                     | 0.51              |
| 48:R:41:SER:HB3   | 48:R:51:GLN:HE21   | 1.75                     | 0.51              |
| 50:T:79:THR:O     | 50:T:82:ILE:HG12   | 2.10                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:A:57:G:H2'      | 53:A:58:C:C6       | 2.46                     | 0.51              |
| 53:A:1054:C:N3     | 58:Y:34:G:H1'      | 2.24                     | 0.51              |
| 53:A:1517:G:C2'    | 53:A:1518:A:H5'    | 2.41                     | 0.51              |
| 54:01:1900:A:O4'   | 54:01:1970:A:H5''  | 2.11                     | 0.51              |
| 59:Z:7:GLN:O       | 59:Z:10:GLU:HB3    | 2.11                     | 0.51              |
| 6:09:90:LEU:HD21   | 6:09:94:ILE:HG23   | 1.92                     | 0.51              |
| 12:15:12:MET:HG2   | 12:15:72:PRO:HG2   | 1.93                     | 0.51              |
| 15:18:24:THR:HA    | 15:18:45:VAL:HG22  | 1.93                     | 0.51              |
| 32:B:102:ASN:ND2   | 32:B:105:THR:HB    | 2.25                     | 0.51              |
| 34:D:40:HIS:C      | 34:D:42:ALA:H      | 2.18                     | 0.51              |
| 35:E:22:LYS:HB3    | 35:E:29:ILE:CG2    | 2.41                     | 0.51              |
| 46:P:5:ARG:NH1     | 46:P:28:ARG:HA     | 2.26                     | 0.51              |
| 47:Q:13:SER:HB3    | 47:Q:21:VAL:CG1    | 2.41                     | 0.51              |
| 53:A:1241:G:H2'    | 53:A:1242:G:H8     | 1.75                     | 0.51              |
| 53:A:1306:A:N6     | 53:A:1331:G:H1'    | 2.25                     | 0.51              |
| 54:01:503:A:H4'    | 54:01:505:A:H5''   | 1.93                     | 0.51              |
| 54:01:827:U:H4'    | 54:01:828:U:C5     | 2.45                     | 0.51              |
| 54:01:1387:A:H2'   | 54:01:1388:G:H8    | 1.75                     | 0.51              |
| 54:01:1434:A:H2'   | 54:01:1435:G:C8    | 2.45                     | 0.51              |
| 54:01:2443:C:H2'   | 54:01:2444:G:H8    | 1.75                     | 0.51              |
| 17:20:49:ILE:HD12  | 17:20:52:PRO:N     | 2.26                     | 0.51              |
| 21:24:44:HIS:NE2   | 21:24:85:LYS:HB2   | 2.26                     | 0.51              |
| 38:H:87:ARG:HD2    | 38:H:89:ASP:OD1    | 2.10                     | 0.51              |
| 44:N:84:ARG:NH2    | 53:A:1059:C:H4'    | 2.26                     | 0.51              |
| 47:Q:11:VAL:CG1    | 47:Q:20:ILE:HD11   | 2.40                     | 0.51              |
| 53:A:1287:A:C2     | 53:A:1353:G:H1'    | 2.44                     | 0.51              |
| 54:01:737:C:O2'    | 54:01:738:G:H5'    | 2.11                     | 0.51              |
| 54:01:1038:G:H2'   | 54:01:1039:A:H8    | 1.75                     | 0.51              |
| 54:01:1563:U:H2'   | 54:01:1564:C:C6    | 2.46                     | 0.51              |
| 54:01:2514:U:H2'   | 54:01:2515:C:C6    | 2.46                     | 0.51              |
| 54:01:2636:C:H2'   | 54:01:2637:U:C6    | 2.45                     | 0.51              |
| 12:15:102:LEU:HD11 | 12:15:126:ILE:HD11 | 1.92                     | 0.51              |
| 15:18:108:ARG:HG2  | 15:18:108:ARG:HH21 | 1.76                     | 0.51              |
| 18:21:11:ARG:O     | 18:21:12:SER:HB2   | 2.10                     | 0.51              |
| 20:23:88:ASP:CG    | 20:23:89:GLY:H     | 2.18                     | 0.51              |
| 33:C:153:SER:HA    | 33:C:164:THR:HG22  | 1.92                     | 0.51              |
| 34:D:61:ARG:HD2    | 34:D:67:LEU:HA     | 1.93                     | 0.51              |
| 35:E:135:VAL:O     | 35:E:138:ALA:HB3   | 2.11                     | 0.51              |
| 39:I:24:ASN:HD22   | 39:I:26:LYS:HB3    | 1.73                     | 0.51              |
| 53:A:1429:A:H2'    | 53:A:1430:A:H8     | 1.76                     | 0.51              |
| 54:01:226:A:H2'    | 54:01:227:A:O4'    | 2.11                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:01:1259:G:H2'  | 54:01:1260:A:H8   | 1.76                     | 0.51              |
| 3:06:148:ILE:HD13 | 3:06:187:VAL:CG1  | 2.41                     | 0.51              |
| 13:16:35:LYS:HG2  | 13:16:110:MET:HE2 | 1.93                     | 0.51              |
| 14:17:31:THR:HG23 | 14:17:32:PRO:HD2  | 1.93                     | 0.51              |
| 28:31:50:GLU:CD   | 28:31:51:ALA:N    | 2.69                     | 0.51              |
| 34:D:31:CYS:SG    | 34:D:33:ILE:HB    | 2.51                     | 0.51              |
| 53:A:323:U:H2'    | 53:A:324:G:O4'    | 2.10                     | 0.51              |
| 54:01:717:C:H2'   | 54:01:718:A:H5'   | 1.92                     | 0.51              |
| 54:01:1331:G:O2'  | 54:01:1332:G:H5'' | 2.10                     | 0.51              |
| 1:04:264:LYS:HD2  | 54:01:2224:G:OP1  | 2.11                     | 0.50              |
| 5:08:163:TYR:HB2  | 5:08:166:GLU:HB2  | 1.93                     | 0.50              |
| 6:09:27:ARG:HD2   | 23:26:55:MET:HE2  | 1.92                     | 0.50              |
| 12:15:27:SER:N    | 12:15:104:GLU:OE2 | 2.44                     | 0.50              |
| 12:15:82:MET:HG3  | 54:01:2250:G:C2   | 2.46                     | 0.50              |
| 14:17:110:ALA:CB  | 14:17:117:PHE:HE2 | 2.23                     | 0.50              |
| 21:24:60:VAL:HA   | 21:24:73:LYS:HG2  | 1.93                     | 0.50              |
| 29:32:13:ASN:O    | 29:32:17:GLY:HA3  | 2.10                     | 0.50              |
| 34:D:26:ALA:HB1   | 34:D:27:ILE:HD12  | 1.92                     | 0.50              |
| 35:E:12:GLU:HA    | 35:E:38:VAL:HG12  | 1.92                     | 0.50              |
| 36:F:5:GLU:HG3    | 36:F:63:ASN:HB2   | 1.93                     | 0.50              |
| 36:F:40:GLU:OE2   | 36:F:61:LEU:HD23  | 2.10                     | 0.50              |
| 37:G:31:VAL:C     | 37:G:33:GLY:H     | 2.18                     | 0.50              |
| 39:I:12:LYS:O     | 39:I:12:LYS:HG2   | 2.10                     | 0.50              |
| 51:U:28:LEU:HD23  | 51:U:28:LEU:C     | 2.35                     | 0.50              |
| 53:A:1299:A:H2'   | 53:A:1300:G:H4'   | 1.93                     | 0.50              |
| 54:01:1139:G:O2'  | 54:01:1140:C:H5'  | 2.12                     | 0.50              |
| 54:01:2112:G:H2'  | 54:01:2113:U:H5'  | 1.93                     | 0.50              |
| 2:05:114:LYS:HG3  | 54:01:2680:U:OP1  | 2.10                     | 0.50              |
| 4:07:28:PRO:CB    | 4:07:168:LEU:HD22 | 2.40                     | 0.50              |
| 8:11:52:LEU:O     | 8:11:54:ILE:HG13  | 2.12                     | 0.50              |
| 9:12:57:LEU:O     | 9:12:58:ASN:HB2   | 2.11                     | 0.50              |
| 20:23:61:GLU:OE1  | 20:23:61:GLU:N    | 2.44                     | 0.50              |
| 32:B:116:LEU:HD12 | 32:B:143:LEU:HD12 | 1.92                     | 0.50              |
| 44:N:2:LYS:HB2    | 44:N:5:MET:HG2    | 1.93                     | 0.50              |
| 46:P:76:LYS:NZ    | 53:A:473:U:H5''   | 2.26                     | 0.50              |
| 47:Q:3:LYS:HG2    | 47:Q:4:ILE:H      | 1.76                     | 0.50              |
| 53:A:26:A:N6      | 53:A:558:G:H1'    | 2.27                     | 0.50              |
| 54:01:616:A:H2'   | 54:01:617:G:O4'   | 2.11                     | 0.50              |
| 54:01:730:A:O2'   | 54:01:731:C:H5'   | 2.11                     | 0.50              |
| 2:05:161:MET:HE1  | 54:01:2050:C:O2   | 2.11                     | 0.50              |
| 3:06:34:ALA:O     | 3:06:37:ALA:HB3   | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:06:71:GLY:HA3   | 54:01:674:G:OP1   | 2.11                     | 0.50              |
| 4:07:30:VAL:HG13  | 4:07:30:VAL:O     | 2.12                     | 0.50              |
| 8:11:7:TYR:CB     | 8:11:59:THR:HA    | 2.42                     | 0.50              |
| 10:13:13:ASN:ND2  | 10:13:98:ARG:HB2  | 2.25                     | 0.50              |
| 15:18:94:ALA:C    | 15:18:95:LYS:HD2  | 2.37                     | 0.50              |
| 22:25:21:ARG:HD2  | 22:25:25:GLU:CD   | 2.37                     | 0.50              |
| 27:30:39:ARG:HH21 | 27:30:39:ARG:HG2  | 1.76                     | 0.50              |
| 42:L:22:ALA:O     | 42:L:26:CYS:SG    | 2.69                     | 0.50              |
| 53:A:163:C:H2'    | 53:A:164:G:O4'    | 2.10                     | 0.50              |
| 54:01:594:U:H2'   | 54:01:595:C:C6    | 2.47                     | 0.50              |
| 54:01:1344:U:H4'  | 54:01:1384:A:N7   | 2.27                     | 0.50              |
| 54:01:1979:U:O2'  | 54:01:1980:G:H5'  | 2.11                     | 0.50              |
| 54:01:2287:A:O2'  | 54:01:2288:A:H2'  | 2.11                     | 0.50              |
| 54:01:2413:G:N2   | 54:01:2414:G:H1'  | 2.26                     | 0.50              |
| 4:07:68:LYS:CD    | 4:07:83:PRO:HD3   | 2.42                     | 0.50              |
| 6:09:25:TYR:O     | 6:09:30:LEU:HG    | 2.12                     | 0.50              |
| 12:15:78:LEU:HD23 | 12:15:78:LEU:C    | 2.37                     | 0.50              |
| 18:21:11:ARG:HH11 | 18:21:11:ARG:HG3  | 1.76                     | 0.50              |
| 34:D:1:ALA:N      | 53:A:405:U:O4     | 2.44                     | 0.50              |
| 34:D:158:LEU:HD23 | 34:D:158:LEU:C    | 2.36                     | 0.50              |
| 35:E:58:ALA:O     | 35:E:61:LYS:HB3   | 2.11                     | 0.50              |
| 38:H:11:THR:HA    | 38:H:14:ARG:NH1   | 2.26                     | 0.50              |
| 38:H:74:ILE:HG23  | 38:H:74:ILE:O     | 2.09                     | 0.50              |
| 44:N:73:LEU:HD13  | 44:N:76:PHE:HD2   | 1.76                     | 0.50              |
| 47:Q:48:GLU:O     | 47:Q:49:ASN:C     | 2.55                     | 0.50              |
| 54:01:254:G:H2'   | 54:01:255:A:H5''  | 1.92                     | 0.50              |
| 54:01:519:U:H2'   | 54:01:520:G:C8    | 2.47                     | 0.50              |
| 54:01:2123:G:N2   | 54:01:2175:C:H42  | 2.08                     | 0.50              |
| 54:01:2128:G:H21  | 54:01:2173:A:H1'  | 1.77                     | 0.50              |
| 54:01:2704:C:H2'  | 54:01:2705:A:O4'  | 2.10                     | 0.50              |
| 1:04:260:LYS:O    | 1:04:262:THR:N    | 2.44                     | 0.50              |
| 13:16:103:ARG:HD2 | 13:16:106:ASP:OD2 | 2.11                     | 0.50              |
| 15:18:20:ARG:HD3  | 15:18:112:ARG:NH1 | 2.24                     | 0.50              |
| 15:18:24:THR:HB   | 15:18:87:ARG:HB2  | 1.94                     | 0.50              |
| 18:21:34:ASP:HB3  | 27:30:27:LEU:CD2  | 2.41                     | 0.50              |
| 34:D:8:LEU:CD2    | 53:A:429:U:H5'    | 2.40                     | 0.50              |
| 37:G:129:ASN:CA   | 37:G:134:VAL:HG11 | 2.38                     | 0.50              |
| 39:I:26:LYS:C     | 39:I:27:ILE:HD12  | 2.37                     | 0.50              |
| 39:I:119:LYS:HE2  | 53:A:1349:A:P     | 2.51                     | 0.50              |
| 51:U:46:ARG:HA    | 51:U:49:ALA:HB3   | 1.93                     | 0.50              |
| 52:03:15:VAL:HG13 | 52:03:21:TYR:HE2  | 1.75                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:01:278:A:H2'   | 54:01:278:A:N3    | 2.26                     | 0.50              |
| 54:01:2485:G:O2'  | 54:01:2486:C:H5'  | 2.11                     | 0.50              |
| 54:01:2808:G:H2'  | 54:01:2890:G:C6   | 2.47                     | 0.50              |
| 7:10:88:HIS:H     | 7:10:89:PRO:HD2   | 1.75                     | 0.50              |
| 12:15:21:ALA:HB2  | 12:15:97:GLN:O    | 2.11                     | 0.50              |
| 13:16:49:GLU:HB2  | 13:16:50:PRO:HD3  | 1.94                     | 0.50              |
| 20:23:9:GLU:HG3   | 20:23:72:PHE:HB3  | 1.93                     | 0.50              |
| 22:25:10:ARG:HH11 | 22:25:10:ARG:HG3  | 1.75                     | 0.50              |
| 22:25:42:HIS:CD2  | 22:25:73:ARG:HD3  | 2.47                     | 0.50              |
| 33:C:38:VAL:HG23  | 33:C:39:ARG:N     | 2.27                     | 0.50              |
| 34:D:131:ILE:HG22 | 34:D:133:SER:H    | 1.76                     | 0.50              |
| 34:D:164:ARG:HG2  | 34:D:165:GLU:N    | 2.25                     | 0.50              |
| 41:K:127:ARG:HG2  | 41:K:127:ARG:HH11 | 1.77                     | 0.50              |
| 53:A:868:C:H2'    | 53:A:869:G:O4'    | 2.11                     | 0.50              |
| 54:01:492:A:H2'   | 54:01:493:G:O4'   | 2.11                     | 0.50              |
| 54:01:1637:A:H5'  | 54:01:1760:C:O2'  | 2.11                     | 0.50              |
| 54:01:2709:G:H2'  | 54:01:2710:C:H6   | 1.75                     | 0.50              |
| 3:06:115:GLN:C    | 3:06:117:ARG:H    | 2.20                     | 0.50              |
| 15:18:30:TRP:CE3  | 15:18:37:LYS:HE3  | 2.46                     | 0.50              |
| 15:18:52:ARG:NE   | 54:01:2845:U:H4'  | 2.26                     | 0.50              |
| 18:21:82:MET:HB3  | 18:21:84:ARG:NH2  | 2.21                     | 0.50              |
| 27:30:9:ARG:HG3   | 27:30:9:ARG:NH2   | 2.27                     | 0.50              |
| 28:31:4:ILE:H     | 28:31:4:ILE:CD1   | 2.21                     | 0.50              |
| 29:32:27:GLY:O    | 29:32:30:VAL:HB   | 2.10                     | 0.50              |
| 30:33:61:LEU:N    | 30:33:62:PRO:HD3  | 2.25                     | 0.50              |
| 36:F:9:MET:HE3    | 36:F:86:ARG:HB2   | 1.93                     | 0.50              |
| 40:J:17:LEU:HD23  | 40:J:17:LEU:C     | 2.37                     | 0.50              |
| 44:N:100:TRP:HZ2  | 53:A:1368:A:H5''  | 1.77                     | 0.50              |
| 51:U:58:LYS:HG3   | 51:U:61:ARG:NE    | 2.25                     | 0.50              |
| 54:01:581:C:H2'   | 54:01:582:A:H8    | 1.76                     | 0.50              |
| 54:01:582:A:H2'   | 54:01:583:G:H8    | 1.75                     | 0.50              |
| 54:01:1055:G:H2'  | 54:01:1056:G:O4'  | 2.11                     | 0.50              |
| 54:01:2443:C:O2'  | 54:01:2444:G:H5'  | 2.12                     | 0.50              |
| 54:01:2691:C:H2'  | 54:01:2692:G:C8   | 2.47                     | 0.50              |
| 59:Z:101:ALA:HB1  | 59:Z:106:GLU:HG2  | 1.94                     | 0.50              |
| 10:13:71:ARG:HH11 | 10:13:71:ARG:HG3  | 1.76                     | 0.50              |
| 13:16:67:PHE:C    | 13:16:69:ARG:H    | 2.19                     | 0.50              |
| 16:19:49:ARG:HG2  | 16:19:49:ARG:NH1  | 2.27                     | 0.50              |
| 20:23:73:ASN:O    | 20:23:74:ALA:HB3  | 2.12                     | 0.50              |
| 24:27:20:ASN:O    | 24:27:25:GLN:HB3  | 2.12                     | 0.50              |
| 25:28:56:VAL:CG2  | 25:28:57:GLU:N    | 2.75                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:D:149:LYS:HG2  | 34:D:150:LYS:HG2   | 1.94                     | 0.50              |
| 35:E:73:VAL:HG11  | 35:E:143:LEU:HB3   | 1.93                     | 0.50              |
| 37:G:39:GLU:HB3   | 37:G:43:TYR:CE2    | 2.47                     | 0.50              |
| 38:H:12:ARG:CD    | 38:H:26:MET:HB3    | 2.41                     | 0.50              |
| 41:K:19:VAL:N     | 41:K:34:THR:O      | 2.44                     | 0.50              |
| 47:Q:45:VAL:HG21  | 47:Q:60:ILE:CD1    | 2.37                     | 0.50              |
| 51:U:28:LEU:O     | 51:U:32:ARG:HB3    | 2.11                     | 0.50              |
| 52:03:214:ILE:O   | 52:03:214:ILE:HG13 | 2.12                     | 0.50              |
| 53:A:423:G:C2'    | 53:A:424:G:H5'     | 2.42                     | 0.50              |
| 53:A:1225:A:H2'   | 53:A:1225:A:N3     | 2.27                     | 0.50              |
| 1:04:131:MET:HA   | 1:04:134:ILE:HD12  | 1.93                     | 0.50              |
| 5:08:44:HIS:O     | 5:08:45:ALA:HB3    | 2.12                     | 0.50              |
| 7:10:113:PHE:CD1  | 7:10:113:PHE:O     | 2.65                     | 0.50              |
| 13:16:31:HIS:CD2  | 54:01:1279:G:H4'   | 2.47                     | 0.50              |
| 29:32:12:ARG:HG3  | 29:32:12:ARG:HH21  | 1.77                     | 0.50              |
| 34:D:58:GLN:O     | 34:D:62:ARG:HG2    | 2.12                     | 0.50              |
| 34:D:171:GLU:HB2  | 34:D:182:LYS:HD2   | 1.93                     | 0.50              |
| 38:H:28:SER:O     | 38:H:29:SER:HB2    | 2.12                     | 0.50              |
| 46:P:40:ASN:HB3   | 46:P:43:ALA:HB2    | 1.92                     | 0.50              |
| 54:01:406:G:H2'   | 54:01:407:G:C8     | 2.47                     | 0.50              |
| 54:01:2082:A:H2'  | 54:01:2083:G:O4'   | 2.12                     | 0.50              |
| 54:01:2293:G:H2'  | 54:01:2294:G:H8    | 1.77                     | 0.50              |
| 54:01:2512:C:H2'  | 54:01:2513:A:O4'   | 2.12                     | 0.50              |
| 59:Z:91:ARG:HA    | 59:Z:94:ALA:HB3    | 1.93                     | 0.50              |
| 1:04:144:GLU:OE1  | 1:04:188:ARG:HB2   | 2.11                     | 0.49              |
| 2:05:124:ARG:HA   | 2:05:165:MET:CE    | 2.41                     | 0.49              |
| 9:12:31:GLU:OE2   | 9:12:34:ARG:HD3    | 2.12                     | 0.49              |
| 10:13:105:ARG:O   | 10:13:107:LEU:N    | 2.45                     | 0.49              |
| 11:14:89:VAL:HG13 | 11:14:89:VAL:O     | 2.12                     | 0.49              |
| 26:29:2:LYS:HB2   | 26:29:5:ILE:CD1    | 2.42                     | 0.49              |
| 34:D:60:VAL:HG21  | 34:D:199:ILE:HD11  | 1.93                     | 0.49              |
| 34:D:187:ARG:NH2  | 34:D:192:ALA:HA    | 2.22                     | 0.49              |
| 40:J:86:ALA:HA    | 40:J:90:LEU:HD12   | 1.94                     | 0.49              |
| 44:N:68:ARG:HG3   | 44:N:69:PRO:HD2    | 1.94                     | 0.49              |
| 46:P:6:LEU:HD13   | 46:P:17:TYR:HB3    | 1.93                     | 0.49              |
| 46:P:19:VAL:HG12  | 46:P:37:GLY:C      | 2.37                     | 0.49              |
| 50:T:14:GLU:C     | 50:T:16:ALA:H      | 2.20                     | 0.49              |
| 53:A:762:U:H2'    | 53:A:763:G:H8      | 1.76                     | 0.49              |
| 54:01:433:C:O2'   | 54:01:434:U:H5'    | 2.12                     | 0.49              |
| 54:01:2419:U:H2'  | 54:01:2420:C:C6    | 2.47                     | 0.49              |
| 3:06:131:THR:HG22 | 3:06:160:ALA:O     | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:10:56:ARG:HB3   | 54:01:1084:A:C1'  | 2.42                     | 0.49              |
| 9:12:113:PRO:HD2  | 54:01:558:U:OP1   | 2.11                     | 0.49              |
| 10:13:40:LYS:NZ   | 10:13:58:LEU:HA   | 2.27                     | 0.49              |
| 19:22:44:LYS:O    | 19:22:48:GLN:HG2  | 2.12                     | 0.49              |
| 25:28:56:VAL:HG22 | 25:28:57:GLU:N    | 2.27                     | 0.49              |
| 34:D:131:ILE:HG12 | 53:A:620:C:N3     | 2.27                     | 0.49              |
| 36:F:22:ILE:O     | 36:F:26:THR:HG22  | 2.12                     | 0.49              |
| 36:F:97:THR:O     | 36:F:98:GLU:HB2   | 2.12                     | 0.49              |
| 37:G:115:MET:HE2  | 53:A:1240:U:N3    | 2.27                     | 0.49              |
| 42:L:21:PRO:C     | 42:L:23:LEU:H     | 2.19                     | 0.49              |
| 52:03:43:ASP:HB2  | 52:03:215:SER:OG  | 2.13                     | 0.49              |
| 53:A:769:G:O2'    | 53:A:770:C:H5'    | 2.12                     | 0.49              |
| 53:A:969:A:H2'    | 53:A:970:C:O4'    | 2.12                     | 0.49              |
| 53:A:1033:G:C3'   | 53:A:1034:G:H5''  | 2.42                     | 0.49              |
| 54:01:30:G:H2'    | 54:01:31:C:C6     | 2.47                     | 0.49              |
| 54:01:2128:G:H2'  | 54:01:2129:C:H5'  | 1.95                     | 0.49              |
| 54:01:2529:G:H5'' | 54:01:2530:A:H5'' | 1.93                     | 0.49              |
| 5:08:2:ARG:NH1    | 54:01:1113:U:H5'  | 2.27                     | 0.49              |
| 7:10:23:LEU:HB3   | 7:10:87:GLU:OE1   | 2.11                     | 0.49              |
| 9:12:16:TYR:CD1   | 9:12:140:LEU:HD22 | 2.47                     | 0.49              |
| 17:20:22:LEU:C    | 17:20:22:LEU:HD12 | 2.37                     | 0.49              |
| 21:24:10:LYS:HG3  | 21:24:11:GLU:N    | 2.26                     | 0.49              |
| 32:B:96:LEU:HB2   | 32:B:99:MET:CG    | 2.43                     | 0.49              |
| 32:B:202:ASN:OD1  | 59:Z:43:LYS:HG2   | 2.12                     | 0.49              |
| 35:E:89:THR:HG21  | 35:E:134:ASN:ND2  | 2.26                     | 0.49              |
| 40:J:9:ARG:HH12   | 40:J:11:LYS:HE3   | 1.76                     | 0.49              |
| 42:L:89:LEU:O     | 42:L:91:GLY:N     | 2.45                     | 0.49              |
| 48:R:41:SER:O     | 48:R:43:ILE:N     | 2.45                     | 0.49              |
| 50:T:31:ILE:HG12  | 50:T:53:MET:HE1   | 1.94                     | 0.49              |
| 51:U:13:VAL:HG22  | 51:U:14:ALA:H     | 1.75                     | 0.49              |
| 54:01:56:A:H2'    | 54:01:57:C:O4'    | 2.13                     | 0.49              |
| 54:01:666:A:H2'   | 54:01:667:U:C6    | 2.48                     | 0.49              |
| 54:01:937:C:H2'   | 54:01:938:G:C8    | 2.46                     | 0.49              |
| 54:01:1370:C:H2'  | 54:01:1371:G:O4'  | 2.12                     | 0.49              |
| 4:07:48:LEU:HA    | 4:07:51:ASN:HD22  | 1.78                     | 0.49              |
| 5:08:8:VAL:O      | 5:08:48:THR:HB    | 2.11                     | 0.49              |
| 8:11:74:PRO:HG2   | 8:11:77:VAL:HG22  | 1.94                     | 0.49              |
| 15:18:52:ARG:HH11 | 15:18:52:ARG:HG3  | 1.77                     | 0.49              |
| 16:19:61:ILE:HG23 | 16:19:75:TYR:CZ   | 2.46                     | 0.49              |
| 18:21:8:ARG:HB3   | 18:21:102:HIS:CE1 | 2.48                     | 0.49              |
| 24:27:39:GLN:HB3  | 24:27:41:HIS:CE1  | 2.47                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:29:5:ILE:HG13  | 26:29:6:HIS:N     | 2.27                     | 0.49              |
| 32:B:110:ILE:O    | 32:B:113:LEU:HB3  | 2.12                     | 0.49              |
| 44:N:7:ALA:C      | 44:N:10:VAL:HG12  | 2.36                     | 0.49              |
| 49:S:28:LYS:HE3   | 49:S:29:PRO:HD2   | 1.95                     | 0.49              |
| 51:U:27:VAL:O     | 51:U:31:VAL:HG12  | 2.12                     | 0.49              |
| 54:01:435:C:C2'   | 54:01:436:C:H5'   | 2.41                     | 0.49              |
| 54:01:633:A:C2'   | 54:01:634:C:H5'   | 2.43                     | 0.49              |
| 54:01:770:G:H2'   | 54:01:771:G:H8    | 1.77                     | 0.49              |
| 54:01:1558:C:H4'  | 54:01:1560:G:OP2  | 2.11                     | 0.49              |
| 54:01:1998:A:H2'  | 54:01:1999:C:C6   | 2.48                     | 0.49              |
| 54:01:2298:A:H2'  | 54:01:2299:U:O4'  | 2.12                     | 0.49              |
| 58:Y:43:C:H2'     | 58:Y:44:G:C8      | 2.48                     | 0.49              |
| 2:05:138:LEU:HD21 | 54:01:745:G:P     | 2.52                     | 0.49              |
| 8:11:90:GLY:O     | 8:11:92:PRO:HD3   | 2.12                     | 0.49              |
| 9:12:58:ASN:ND2   | 9:12:128:ASN:HB2  | 2.25                     | 0.49              |
| 12:15:4:PRO:HG2   | 12:15:92:TRP:CE3  | 2.47                     | 0.49              |
| 16:19:60:TRP:HZ2  | 54:01:995:C:H1'   | 1.77                     | 0.49              |
| 24:27:24:GLU:O    | 24:27:25:GLN:C    | 2.55                     | 0.49              |
| 28:31:36:LYS:HA   | 28:31:46:VAL:O    | 2.13                     | 0.49              |
| 31:34:3:VAL:HG23  | 31:34:3:VAL:O     | 2.13                     | 0.49              |
| 43:M:3:ILE:HG22   | 43:M:56:ARG:CZ    | 2.42                     | 0.49              |
| 50:T:53:MET:C     | 50:T:55:PRO:HD2   | 2.36                     | 0.49              |
| 53:A:1074:G:H2'   | 53:A:1075:U:H6    | 1.76                     | 0.49              |
| 54:01:181:A:H2'   | 54:01:182:A:C8    | 2.47                     | 0.49              |
| 54:01:1595:C:H2'  | 54:01:1596:A:H8   | 1.78                     | 0.49              |
| 54:01:2204:G:H2'  | 54:01:2205:A:H8   | 1.76                     | 0.49              |
| 54:01:2286:G:H4'  | 54:01:2287:A:O4'  | 2.12                     | 0.49              |
| 54:01:2799:A:C2'  | 54:01:2800:A:H5'  | 2.43                     | 0.49              |
| 55:02:97:C:H2'    | 55:02:98:G:H5'    | 1.94                     | 0.49              |
| 2:05:61:THR:HB    | 54:01:2811:G:OP1  | 2.13                     | 0.49              |
| 5:08:102:ILE:HD11 | 5:08:116:LEU:CD2  | 2.43                     | 0.49              |
| 7:10:108:VAL:HG12 | 7:10:109:LYS:N    | 2.27                     | 0.49              |
| 19:22:45:ALA:O    | 19:22:49:LYS:HD3  | 2.12                     | 0.49              |
| 23:26:7:THR:OG1   | 23:26:9:LYS:HG3   | 2.13                     | 0.49              |
| 27:30:2:VAL:HG12  | 27:30:3:GLN:N     | 2.28                     | 0.49              |
| 33:C:113:LYS:N    | 33:C:184:ASN:HD22 | 2.10                     | 0.49              |
| 36:F:72:ASP:O     | 36:F:75:GLU:HB3   | 2.13                     | 0.49              |
| 45:O:28:VAL:HG11  | 45:O:66:LEU:HD21  | 1.94                     | 0.49              |
| 53:A:229:U:H2'    | 53:A:230:G:H8     | 1.76                     | 0.49              |
| 53:A:721:G:H4'    | 53:A:722:G:O4'    | 2.12                     | 0.49              |
| 53:A:1259:C:H3'   | 53:A:1260:G:C5'   | 2.29                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 54:01:458:G:O2'  | 54:01:459:U:H5    | 1.96                     | 0.49              |
| 54:01:548:G:H2'  | 54:01:549:G:O4'   | 2.12                     | 0.49              |
| 54:01:1409:U:H2' | 54:01:1410:G:C8   | 2.47                     | 0.49              |
| 54:01:1779:U:OP2 | 54:01:1784:A:N6   | 2.45                     | 0.49              |
| 54:01:2648:G:H2' | 54:01:2649:C:H6   | 1.78                     | 0.49              |
| 55:02:30:C:H2'   | 55:02:31:C:H5'    | 1.95                     | 0.49              |
| 1:04:89:ASN:N    | 1:04:89:ASN:HD22  | 2.10                     | 0.49              |
| 9:12:25:LEU:HB3  | 54:01:1140:C:OP1  | 2.13                     | 0.49              |
| 11:14:78:ARG:HB3 | 11:14:113:ALA:HB2 | 1.95                     | 0.49              |
| 15:18:19:PHE:CE2 | 15:18:83:ILE:HG21 | 2.48                     | 0.49              |
| 15:18:74:GLN:HB2 | 15:18:77:SER:HB2  | 1.93                     | 0.49              |
| 18:21:84:ARG:HB2 | 18:21:96:ILE:HG13 | 1.95                     | 0.49              |
| 27:30:11:LYS:HA  | 27:30:14:MET:HE3  | 1.94                     | 0.49              |
| 32:B:6:ARG:HG2   | 32:B:6:ARG:HH11   | 1.78                     | 0.49              |
| 34:D:87:GLU:N    | 34:D:87:GLU:OE1   | 2.46                     | 0.49              |
| 39:I:30:ASN:HD21 | 39:I:65:THR:HA    | 1.78                     | 0.49              |
| 39:I:38:PHE:C    | 39:I:38:PHE:CD1   | 2.90                     | 0.49              |
| 53:A:1487:G:O2'  | 53:A:1488:G:H5'   | 2.12                     | 0.49              |
| 54:01:1373:A:C5' | 54:01:2212:A:H1'  | 2.40                     | 0.49              |
| 54:01:1971:U:H5' | 54:01:1972:G:H5'' | 1.95                     | 0.49              |
| 54:01:2190:G:H2' | 54:01:2191:A:C8   | 2.48                     | 0.49              |
| 1:04:83:ASP:HB2  | 1:04:90:ILE:HG12  | 1.94                     | 0.49              |
| 3:06:134:LEU:CD2 | 3:06:161:ALA:HB2  | 2.42                     | 0.49              |
| 4:07:167:ALA:O   | 4:07:170:ALA:HB3  | 2.13                     | 0.49              |
| 6:09:1:MET:O     | 6:09:20:ASN:HA    | 2.13                     | 0.49              |
| 7:10:28:ALA:HB2  | 7:10:81:LEU:O     | 2.13                     | 0.49              |
| 8:11:57:VAL:O    | 8:11:68:PHE:HA    | 2.12                     | 0.49              |
| 24:27:31:GLN:HG3 | 24:27:36:GLN:HB2  | 1.95                     | 0.49              |
| 28:31:39:ASP:OD1 | 28:31:40:PRO:HD2  | 2.13                     | 0.49              |
| 37:G:71:THR:HA   | 37:G:95:ARG:HH12  | 1.78                     | 0.49              |
| 42:L:47:ALA:C    | 42:L:48:LEU:HD12  | 2.37                     | 0.49              |
| 43:M:52:ILE:HG22 | 43:M:56:ARG:HH12  | 1.77                     | 0.49              |
| 46:P:6:LEU:HD13  | 46:P:17:TYR:CB    | 2.42                     | 0.49              |
| 49:S:20:LYS:HA   | 49:S:23:GLU:OE2   | 2.12                     | 0.49              |
| 51:U:62:GLU:HG2  | 51:U:62:GLU:O     | 2.12                     | 0.49              |
| 53:A:195:A:H2'   | 53:A:196:A:C8     | 2.48                     | 0.49              |
| 53:A:880:C:H2'   | 53:A:881:G:C8     | 2.48                     | 0.49              |
| 53:A:1259:C:C3'  | 53:A:1260:G:H5''  | 2.32                     | 0.49              |
| 53:A:1368:A:O2'  | 53:A:1369:C:H5'   | 2.12                     | 0.49              |
| 54:01:189:G:H2'  | 54:01:205:G:N2    | 2.28                     | 0.49              |
| 54:01:437:U:H2'  | 54:01:438:G:H8    | 1.78                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 54:01:1409:U:H2'  | 54:01:1410:G:H8    | 1.78                     | 0.49              |
| 54:01:1528:A:H2'  | 54:01:1529:G:O4'   | 2.12                     | 0.49              |
| 54:01:2469:A:H2'  | 54:01:2470:G:O4'   | 2.13                     | 0.49              |
| 4:07:68:LYS:HD3   | 4:07:83:PRO:HD3    | 1.95                     | 0.49              |
| 8:11:13:ALA:HA    | 8:11:53:PRO:HA     | 1.95                     | 0.49              |
| 12:15:66:ARG:HG3  | 12:15:66:ARG:HH11  | 1.78                     | 0.49              |
| 17:20:22:LEU:HD12 | 17:20:23:GLU:O     | 2.12                     | 0.49              |
| 18:21:6:LYS:HB2   | 18:21:103:ILE:O    | 2.13                     | 0.49              |
| 19:22:74:ILE:HG13 | 19:22:74:ILE:O     | 2.12                     | 0.49              |
| 20:23:95:PHE:CE2  | 20:23:102:ILE:HG12 | 2.47                     | 0.49              |
| 21:24:26:PHE:CE1  | 21:24:42:LEU:HD11  | 2.47                     | 0.49              |
| 25:28:19:HIS:O    | 25:28:20:LYS:C     | 2.55                     | 0.49              |
| 27:30:2:VAL:HG22  | 54:01:2015:A:C2    | 2.48                     | 0.49              |
| 30:33:25:HIS:HB3  | 30:33:43:LEU:HD22  | 1.93                     | 0.49              |
| 34:D:140:ASP:H    | 34:D:181:PHE:HB3   | 1.78                     | 0.49              |
| 39:I:17:ARG:O     | 39:I:64:ILE:HG23   | 2.11                     | 0.49              |
| 40:J:67:ILE:HG23  | 44:N:95:LEU:HD13   | 1.94                     | 0.49              |
| 51:U:48:LYS:HA    | 51:U:51:ALA:CB     | 2.42                     | 0.49              |
| 52:03:183:ASP:O   | 52:03:187:GLU:HG2  | 2.13                     | 0.49              |
| 53:A:437:U:O2'    | 53:A:438:U:H5'     | 2.12                     | 0.49              |
| 53:A:902:G:H2'    | 53:A:903:G:H8      | 1.78                     | 0.49              |
| 53:A:1349:A:H2'   | 53:A:1350:A:O4'    | 2.13                     | 0.49              |
| 54:01:776:G:H1    | 54:01:2072:C:H5'   | 1.76                     | 0.49              |
| 54:01:1259:G:H2'  | 54:01:1260:A:C8    | 2.48                     | 0.49              |
| 54:01:1415:U:H2'  | 54:01:1416:G:H4'   | 1.95                     | 0.49              |
| 54:01:2533:U:H2'  | 54:01:2534:A:O4'   | 2.13                     | 0.49              |
| 54:01:2730:C:H2'  | 54:01:2731:G:H8    | 1.77                     | 0.49              |
| 1:04:56:GLY:HA2   | 1:04:212:TRP:HA    | 1.95                     | 0.49              |
| 2:05:9:VAL:HA     | 2:05:197:THR:HG23  | 1.95                     | 0.49              |
| 3:06:105:LEU:HA   | 3:06:108:ILE:HD12  | 1.93                     | 0.49              |
| 4:07:87:LYS:HD2   | 54:01:2313:C:H5''  | 1.95                     | 0.49              |
| 5:08:3:VAL:HG21   | 54:01:2748:A:H5'   | 1.94                     | 0.49              |
| 7:10:103:ASN:HA   | 7:10:107:GLU:OE1   | 2.13                     | 0.49              |
| 17:20:1:MET:H1    | 17:20:43:ASN:HA    | 1.78                     | 0.49              |
| 29:32:22:MET:SD   | 29:32:28:ARG:HG2   | 2.53                     | 0.49              |
| 32:B:100:LEU:HB3  | 32:B:178:LEU:HD12  | 1.95                     | 0.49              |
| 32:B:185:ILE:HD13 | 32:B:199:ILE:HB    | 1.94                     | 0.49              |
| 33:C:155:ARG:O    | 33:C:156:LEU:C     | 2.55                     | 0.49              |
| 34:D:117:VAL:HG22 | 34:D:122:ILE:HG13  | 1.95                     | 0.49              |
| 36:F:15:SER:HA    | 36:F:18:VAL:CG2    | 2.43                     | 0.49              |
| 37:G:6:ILE:HD12   | 37:G:6:ILE:C       | 2.37                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:I:114:LYS:HG2  | 39:I:120:ALA:O     | 2.13                     | 0.49              |
| 42:L:73:LEU:N     | 42:L:73:LEU:HD12   | 2.27                     | 0.49              |
| 52:03:6:LYS:HG3   | 52:03:7:ARG:N      | 2.26                     | 0.49              |
| 53:A:1527:U:H2'   | 53:A:1528:U:C6     | 2.48                     | 0.49              |
| 54:01:189:G:H2'   | 54:01:205:G:H22    | 1.78                     | 0.49              |
| 54:01:543:G:H5'   | 54:01:543:G:H8     | 1.78                     | 0.49              |
| 54:01:727:A:O2'   | 54:01:728:G:H5'    | 2.12                     | 0.49              |
| 54:01:886:A:H2'   | 54:01:887:U:H4'    | 1.95                     | 0.49              |
| 54:01:968:C:H2'   | 54:01:969:G:H8     | 1.78                     | 0.49              |
| 54:01:1346:G:H2'  | 54:01:1347:A:H8    | 1.78                     | 0.49              |
| 54:01:1704:C:H2'  | 54:01:1705:A:C8    | 2.47                     | 0.49              |
| 54:01:2042:A:H2'  | 54:01:2043:C:H5'   | 1.95                     | 0.49              |
| 54:01:2215:C:H2'  | 54:01:2216:G:C8    | 2.48                     | 0.49              |
| 54:01:2267:A:H5'' | 54:01:2268:A:H5'   | 1.95                     | 0.49              |
| 1:04:8:THR:HG21   | 54:01:727:A:H2     | 1.77                     | 0.48              |
| 1:04:131:MET:HA   | 1:04:134:ILE:CD1   | 2.43                     | 0.48              |
| 5:08:126:THR:HG22 | 5:08:128:THR:H     | 1.77                     | 0.48              |
| 6:09:68:ARG:O     | 6:09:72:ILE:HG13   | 2.13                     | 0.48              |
| 12:15:55:ARG:HD3  | 54:01:2469:A:H4'   | 1.95                     | 0.48              |
| 13:16:67:PHE:C    | 13:16:69:ARG:N     | 2.70                     | 0.48              |
| 14:17:68:LYS:HA   | 14:17:102:ARG:HG2  | 1.94                     | 0.48              |
| 15:18:7:LEU:HA    | 15:18:10:GLU:OE2   | 2.13                     | 0.48              |
| 16:19:101:ASP:OD2 | 16:19:104:ALA:HB2  | 2.13                     | 0.48              |
| 18:21:1:MET:H2    | 18:21:110:ARG:HH11 | 1.61                     | 0.48              |
| 26:29:37:CYS:HG   | 26:29:40:CYS:CB    | 2.26                     | 0.48              |
| 35:E:80:LEU:HG    | 35:E:146:MET:SD    | 2.53                     | 0.48              |
| 45:O:36:ASN:HA    | 45:O:39:GLN:HG2    | 1.95                     | 0.48              |
| 53:A:1071:C:H2'   | 53:A:1072:G:C8     | 2.48                     | 0.48              |
| 53:A:1074:G:H2'   | 53:A:1075:U:C6     | 2.48                     | 0.48              |
| 54:01:1507:C:H2'  | 54:01:1508:A:O4'   | 2.13                     | 0.48              |
| 54:01:2436:G:H2'  | 54:01:2437:G:H8    | 1.77                     | 0.48              |
| 54:01:2450:A:OP1  | 54:01:2497:A:H2'   | 2.12                     | 0.48              |
| 54:01:2694:G:H2'  | 54:01:2695:U:C6    | 2.47                     | 0.48              |
| 54:01:2715:C:C2'  | 54:01:2716:C:H5''  | 2.43                     | 0.48              |
| 55:02:63:C:H2'    | 55:02:64:G:H8      | 1.78                     | 0.48              |
| 3:06:48:THR:O     | 3:06:52:VAL:HG23   | 2.13                     | 0.48              |
| 6:09:18:GLN:HE22  | 6:09:44:ILE:HD13   | 1.77                     | 0.48              |
| 8:11:51:GLY:C     | 8:11:52:LEU:HD12   | 2.38                     | 0.48              |
| 9:12:41:LYS:HB3   | 9:12:43:GLU:OE1    | 2.13                     | 0.48              |
| 13:16:24:MET:HE3  | 13:16:44:LEU:HD13  | 1.95                     | 0.48              |
| 14:17:34:HIS:HA   | 14:17:53:THR:OG1   | 2.13                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:17:101:GLY:O    | 14:17:104:GLN:N   | 2.46                     | 0.48              |
| 29:32:8:SER:O      | 29:32:9:VAL:C     | 2.56                     | 0.48              |
| 31:34:31:PRO:O     | 31:34:34:LYS:HB3  | 2.12                     | 0.48              |
| 35:E:22:LYS:HB3    | 35:E:29:ILE:HG23  | 1.94                     | 0.48              |
| 39:I:96:GLU:N      | 39:I:96:GLU:OE1   | 2.46                     | 0.48              |
| 40:J:53:ILE:HG22   | 40:J:61:ALA:O     | 2.13                     | 0.48              |
| 41:K:112:VAL:O     | 41:K:113:THR:C    | 2.55                     | 0.48              |
| 51:U:25:ALA:O      | 51:U:26:GLY:C     | 2.56                     | 0.48              |
| 52:03:213:SER:HA   | 52:03:222:VAL:O   | 2.13                     | 0.48              |
| 53:A:33:A:H2'      | 53:A:34:C:C6      | 2.48                     | 0.48              |
| 54:01:437:U:H2'    | 54:01:438:G:C8    | 2.48                     | 0.48              |
| 54:01:1204:A:H4'   | 54:01:1205:A:H5'' | 1.95                     | 0.48              |
| 54:01:1364:G:H5'   | 54:01:1809:A:H1'  | 1.95                     | 0.48              |
| 54:01:1883:U:H2'   | 54:01:1884:G:O4'  | 2.13                     | 0.48              |
| 55:02:79:G:H2'     | 55:02:80:U:O4'    | 2.13                     | 0.48              |
| 58:Y:47:U:H3'      | 58:Y:48:C:H5''    | 1.95                     | 0.48              |
| 1:04:42:ARG:HH11   | 1:04:42:ARG:HG3   | 1.78                     | 0.48              |
| 1:04:237:ARG:HD2   | 54:01:2591:C:OP1  | 2.13                     | 0.48              |
| 4:07:82:TYR:CD1    | 4:07:83:PRO:HD2   | 2.48                     | 0.48              |
| 18:21:107:VAL:HG13 | 18:21:107:VAL:O   | 2.12                     | 0.48              |
| 20:23:4:ILE:N      | 20:23:4:ILE:CD1   | 2.77                     | 0.48              |
| 23:26:69:GLU:O     | 23:26:72:ALA:HB3  | 2.14                     | 0.48              |
| 33:C:86:LEU:O      | 33:C:90:VAL:HG23  | 2.14                     | 0.48              |
| 37:G:55:LYS:HB2    | 37:G:60:ALA:HB2   | 1.95                     | 0.48              |
| 39:I:110:VAL:O     | 39:I:110:VAL:HG23 | 2.12                     | 0.48              |
| 41:K:23:HIS:HB3    | 41:K:30:ILE:CG2   | 2.43                     | 0.48              |
| 45:O:55:LEU:O      | 45:O:58:MET:HG2   | 2.13                     | 0.48              |
| 50:T:23:ARG:HH21   | 50:T:60:GLN:HE22  | 1.60                     | 0.48              |
| 53:A:1251:A:H2'    | 53:A:1252:A:C8    | 2.47                     | 0.48              |
| 54:01:531:C:O2'    | 54:01:563:A:H5''  | 2.14                     | 0.48              |
| 54:01:1219:U:H2'   | 54:01:1220:G:C8   | 2.48                     | 0.48              |
| 54:01:2564:A:C2    | 54:01:2647:U:H4'  | 2.49                     | 0.48              |
| 55:02:104:A:H2'    | 55:02:105:G:O4'   | 2.14                     | 0.48              |
| 56:W:50:U:H2'      | 56:W:51:C:C6      | 2.47                     | 0.48              |
| 1:04:12:ARG:HD3    | 1:04:15:VAL:HG21  | 1.95                     | 0.48              |
| 6:09:117:LEU:O     | 6:09:119:ASN:N    | 2.44                     | 0.48              |
| 9:12:14:ASP:CG     | 9:12:15:TRP:H     | 2.22                     | 0.48              |
| 13:16:73:ASN:HA    | 13:16:76:VAL:HG12 | 1.95                     | 0.48              |
| 21:24:51:GLN:OE1   | 21:24:86:LEU:HD21 | 2.14                     | 0.48              |
| 31:34:26:ILE:HD12  | 31:34:26:ILE:C    | 2.38                     | 0.48              |
| 42:L:28:GLN:HB3    | 42:L:80:LEU:HD11  | 1.94                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 42:L:86:VAL:CG2  | 42:L:89:LEU:H     | 2.26                     | 0.48              |
| 46:P:14:ARG:NH2  | 46:P:42:ILE:HD12  | 2.28                     | 0.48              |
| 51:U:36:PHE:O    | 51:U:37:TYR:HB3   | 2.12                     | 0.48              |
| 53:A:128:G:O2'   | 53:A:129:A:H5'    | 2.13                     | 0.48              |
| 53:A:206:C:H2'   | 53:A:207:C:O4'    | 2.14                     | 0.48              |
| 53:A:236:A:H2'   | 53:A:237:G:H8     | 1.77                     | 0.48              |
| 53:A:674:G:H2'   | 53:A:675:A:C8     | 2.48                     | 0.48              |
| 7:10:54:VAL:HG22 | 7:10:54:VAL:O     | 2.12                     | 0.48              |
| 22:25:42:HIS:HB2 | 22:25:75:PHE:CD1  | 2.48                     | 0.48              |
| 27:30:52:LYS:HG3 | 27:30:52:LYS:O    | 2.13                     | 0.48              |
| 32:B:212:TYR:O   | 32:B:216:VAL:HG23 | 2.12                     | 0.48              |
| 33:C:38:VAL:O    | 33:C:42:LEU:HD13  | 2.14                     | 0.48              |
| 33:C:72:PRO:HG3  | 33:C:104:GLU:CD   | 2.38                     | 0.48              |
| 36:F:86:ARG:NH2  | 53:A:673:A:O3'    | 2.46                     | 0.48              |
| 37:G:44:SER:HA   | 37:G:47:GLU:OE1   | 2.13                     | 0.48              |
| 37:G:135:LYS:O   | 37:G:138:GLU:HB2  | 2.14                     | 0.48              |
| 40:J:53:ILE:HG23 | 53:A:1060:U:H4'   | 1.96                     | 0.48              |
| 43:M:1:ALA:H1    | 43:M:52:ILE:HD13  | 1.79                     | 0.48              |
| 47:Q:39:ARG:HG3  | 47:Q:39:ARG:HH11  | 1.79                     | 0.48              |
| 54:01:406:G:H2'  | 54:01:407:G:H8    | 1.77                     | 0.48              |
| 54:01:542:C:H2'  | 54:01:543:G:C5'   | 2.44                     | 0.48              |
| 54:01:572:A:H5'' | 54:01:573:U:OP2   | 2.13                     | 0.48              |
| 54:01:1565:C:O2' | 54:01:1566:A:H2'  | 2.14                     | 0.48              |
| 54:01:1595:C:H2' | 54:01:1596:A:C8   | 2.48                     | 0.48              |
| 54:01:2415:G:H2' | 54:01:2416:C:C6   | 2.49                     | 0.48              |
| 54:01:2648:G:H2' | 54:01:2649:C:C6   | 2.48                     | 0.48              |
| 54:01:2718:G:H21 | 54:01:2847:U:H4'  | 1.78                     | 0.48              |
| 55:02:72:G:H21   | 55:02:104:A:H62   | 1.61                     | 0.48              |
| 4:07:99:PHE:O    | 4:07:103:ILE:HG23 | 2.14                     | 0.48              |
| 4:07:141:ASP:O   | 4:07:142:TYR:HB3  | 2.13                     | 0.48              |
| 5:08:9:VAL:O     | 5:08:9:VAL:HG13   | 2.13                     | 0.48              |
| 8:11:124:MET:O   | 8:11:127:SER:HB3  | 2.13                     | 0.48              |
| 13:16:99:LYS:HE2 | 27:30:40:HIS:O    | 2.14                     | 0.48              |
| 14:17:17:LYS:HZ3 | 54:01:2380:C:H5'  | 1.77                     | 0.48              |
| 15:18:96:LEU:O   | 15:18:98:TYR:N    | 2.46                     | 0.48              |
| 32:B:47:PRO:HA   | 32:B:50:ASN:HD22  | 1.78                     | 0.48              |
| 39:I:43:ALA:O    | 39:I:46:VAL:HG13  | 2.13                     | 0.48              |
| 47:Q:13:SER:H    | 47:Q:21:VAL:CG1   | 2.24                     | 0.48              |
| 50:T:14:GLU:C    | 50:T:16:ALA:N     | 2.71                     | 0.48              |
| 53:A:1109:C:H2'  | 53:A:1110:A:O4'   | 2.13                     | 0.48              |
| 54:01:2314:A:H2' | 54:01:2315:G:C8   | 2.49                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:06:5:LEU:HD22  | 3:06:10:SER:HB3   | 1.94                     | 0.48              |
| 5:08:3:VAL:HG22  | 54:01:2751:G:H4'  | 1.95                     | 0.48              |
| 6:09:117:LEU:C   | 6:09:119:ASN:H    | 2.21                     | 0.48              |
| 7:10:55:VAL:HA   | 54:01:1084:A:H5'' | 1.94                     | 0.48              |
| 7:10:60:LEU:HG   | 7:10:78:GLY:HA3   | 1.95                     | 0.48              |
| 32:B:202:ASN:HB2 | 59:Z:43:LYS:HZ1   | 1.76                     | 0.48              |
| 36:F:51:ILE:HG23 | 36:F:86:ARG:HE    | 1.79                     | 0.48              |
| 37:G:14:ASP:OD2  | 37:G:16:LYS:HB3   | 2.13                     | 0.48              |
| 44:N:20:PHE:C    | 44:N:22:LYS:H     | 2.20                     | 0.48              |
| 50:T:54:GLN:O    | 50:T:57:VAL:HG12  | 2.14                     | 0.48              |
| 53:A:1414:U:H2'  | 53:A:1415:G:H8    | 1.79                     | 0.48              |
| 54:01:873:C:H2'  | 54:01:874:G:H8    | 1.77                     | 0.48              |
| 54:01:2055:C:H2' | 54:01:2504:U:H5'  | 1.96                     | 0.48              |
| 54:01:2266:A:H4' | 54:01:2267:A:N3   | 2.28                     | 0.48              |
| 55:02:97:C:C2'   | 55:02:98:G:H5'    | 2.44                     | 0.48              |
| 1:04:151:GLY:C   | 1:04:152:GLN:HG2  | 2.39                     | 0.48              |
| 5:08:66:THR:HG23 | 54:01:2747:G:O2'  | 2.13                     | 0.48              |
| 26:29:36:VAL:HB  | 26:29:40:CYS:SG   | 2.53                     | 0.48              |
| 37:G:102:TRP:CH2 | 37:G:140:VAL:HG21 | 2.49                     | 0.48              |
| 42:L:32:VAL:O    | 42:L:33:CYS:HB3   | 2.13                     | 0.48              |
| 42:L:34:THR:N    | 42:L:53:ARG:O     | 2.44                     | 0.48              |
| 45:O:81:ILE:HG13 | 45:O:82:GLU:N     | 2.29                     | 0.48              |
| 46:P:14:ARG:HH11 | 46:P:14:ARG:HG3   | 1.79                     | 0.48              |
| 46:P:40:ASN:OD1  | 46:P:43:ALA:N     | 2.47                     | 0.48              |
| 46:P:48:GLU:CG   | 46:P:49:GLY:H     | 2.16                     | 0.48              |
| 50:T:70:LYS:HA   | 50:T:73:ARG:NH1   | 2.29                     | 0.48              |
| 53:A:422:C:H5'   | 53:A:423:G:N3     | 2.28                     | 0.48              |
| 53:A:580:C:H2'   | 53:A:581:G:O4'    | 2.14                     | 0.48              |
| 53:A:608:A:H2'   | 53:A:609:A:C8     | 2.48                     | 0.48              |
| 53:A:1171:A:H2'  | 53:A:1172:C:C6    | 2.49                     | 0.48              |
| 54:01:611:C:H2'  | 54:01:612:G:O4'   | 2.14                     | 0.48              |
| 54:01:2361:G:O2' | 54:01:2362:C:H5'  | 2.13                     | 0.48              |
| 55:02:49:C:H2'   | 55:02:50:A:H8     | 1.79                     | 0.48              |
| 55:02:106:G:H2'  | 55:02:107:G:O4'   | 2.14                     | 0.48              |
| 5:08:98:LYS:HZ2  | 5:08:103:ASN:HD22 | 1.62                     | 0.48              |
| 6:09:12:LEU:C    | 6:09:12:LEU:HD12  | 2.38                     | 0.48              |
| 6:09:31:VAL:N    | 6:09:32:PRO:HD2   | 2.28                     | 0.48              |
| 8:11:85:ILE:HD12 | 8:11:85:ILE:C     | 2.38                     | 0.48              |
| 11:14:58:TYR:CD1 | 11:14:59:ARG:N    | 2.82                     | 0.48              |
| 12:15:41:LEU:HG  | 12:15:96:ILE:HG13 | 1.95                     | 0.48              |
| 13:16:3:HIS:O    | 13:16:4:ARG:HB2   | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:31:36:LYS:CG   | 28:31:45:HIS:HB3  | 2.43                     | 0.48              |
| 29:32:10:LEU:O    | 29:32:14:ARG:HG2  | 2.13                     | 0.48              |
| 34:D:202:LEU:HD23 | 34:D:202:LEU:C    | 2.38                     | 0.48              |
| 39:I:129:ARG:HG2  | 39:I:129:ARG:HH11 | 1.78                     | 0.48              |
| 43:M:6:ILE:HG13   | 43:M:7:ASN:N      | 2.21                     | 0.48              |
| 46:P:8:ARG:HB3    | 46:P:28:ARG:CZ    | 2.44                     | 0.48              |
| 50:T:23:ARG:HH22  | 50:T:63:LYS:NZ    | 2.09                     | 0.48              |
| 51:U:39:LYS:N     | 51:U:40:PRO:CD    | 2.77                     | 0.48              |
| 53:A:82:G:H1      | 53:A:87:C:H42     | 1.62                     | 0.48              |
| 53:A:131:A:H2'    | 53:A:132:C:C6     | 2.49                     | 0.48              |
| 53:A:744:C:H2'    | 53:A:745:G:H8     | 1.79                     | 0.48              |
| 54:01:65:U:H2'    | 54:01:66:C:C6     | 2.49                     | 0.48              |
| 54:01:304:U:H2'   | 54:01:305:C:C6    | 2.48                     | 0.48              |
| 54:01:2086:U:H2'  | 54:01:2087:G:H8   | 1.78                     | 0.48              |
| 59:Z:33:LYS:O     | 59:Z:34:ASP:HB2   | 2.14                     | 0.48              |
| 1:04:104:LEU:HD12 | 1:04:142:ASN:HB2  | 1.95                     | 0.48              |
| 3:06:63:LYS:HZ1   | 54:01:2060:A:H3'  | 1.78                     | 0.48              |
| 4:07:139:GLU:H    | 4:07:139:GLU:CD   | 2.22                     | 0.48              |
| 6:09:125:THR:HG23 | 6:09:146:VAL:O    | 2.14                     | 0.48              |
| 12:15:26:VAL:HA   | 12:15:104:GLU:OE2 | 2.14                     | 0.48              |
| 15:18:23:ASP:O    | 15:18:25:VAL:HG23 | 2.14                     | 0.48              |
| 18:21:21:ALA:O    | 18:21:25:ARG:HG2  | 2.14                     | 0.48              |
| 25:28:30:ARG:HG2  | 25:28:30:ARG:HH11 | 1.79                     | 0.48              |
| 33:C:22:PHE:CE2   | 40:J:11:LYS:HG3   | 2.49                     | 0.48              |
| 34:D:50:TYR:CD2   | 53:A:508:U:H4'    | 2.49                     | 0.48              |
| 53:A:494:G:O2'    | 53:A:496:A:H1'    | 2.14                     | 0.48              |
| 53:A:762:U:H2'    | 53:A:763:G:C8     | 2.49                     | 0.48              |
| 54:01:230:G:O2'   | 54:01:231:A:H5'   | 2.14                     | 0.48              |
| 54:01:248:G:H3'   | 54:01:249:C:C5'   | 2.44                     | 0.48              |
| 54:01:2183:A:H2'  | 54:01:2184:A:H8   | 1.79                     | 0.48              |
| 2:05:125:TRP:CG   | 2:05:160:LYS:HB3  | 2.49                     | 0.47              |
| 4:07:101:ARG:HG3  | 4:07:105:ILE:HD11 | 1.96                     | 0.47              |
| 4:07:122:ASP:OD2  | 4:07:124:ARG:HB3  | 2.14                     | 0.47              |
| 11:14:93:ASN:O    | 11:14:94:THR:HB   | 2.14                     | 0.47              |
| 15:18:59:THR:HG22 | 15:18:72:VAL:CG1  | 2.24                     | 0.47              |
| 17:20:37:GLU:HA   | 17:20:53:PHE:CD1  | 2.49                     | 0.47              |
| 25:28:57:GLU:HG3  | 25:28:57:GLU:O    | 2.14                     | 0.47              |
| 34:D:5:GLY:O      | 34:D:7:LYS:N      | 2.47                     | 0.47              |
| 35:E:54:GLU:HG2   | 35:E:56:PRO:CD    | 2.40                     | 0.47              |
| 36:F:100:SER:HB3  | 36:F:101:PRO:CD   | 2.44                     | 0.47              |
| 42:L:48:LEU:HB2   | 53:A:520:A:OP1    | 2.13                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:L:83:GLY:HA3   | 53:A:552:U:O3'    | 2.14                     | 0.47              |
| 53:A:405:U:C3'    | 53:A:406:G:H5'    | 2.40                     | 0.47              |
| 53:A:1052:U:H2'   | 53:A:1200:C:H41   | 1.78                     | 0.47              |
| 54:01:1035:U:H2'  | 54:01:1036:G:H8   | 1.78                     | 0.47              |
| 54:01:1387:A:H2'  | 54:01:1388:G:C8   | 2.49                     | 0.47              |
| 54:01:2371:G:O2'  | 54:01:2372:U:H5'  | 2.14                     | 0.47              |
| 54:01:2741:A:H2'  | 54:01:2742:G:O4'  | 2.14                     | 0.47              |
| 56:W:47:U:H3'     | 56:W:48:C:C5'     | 2.44                     | 0.47              |
| 58:Y:47:U:H3'     | 58:Y:48:C:C5'     | 2.44                     | 0.47              |
| 2:05:150:GLN:HB2  | 54:01:2572:A:N7   | 2.30                     | 0.47              |
| 6:09:132:PHE:N    | 6:09:140:ALA:O    | 2.47                     | 0.47              |
| 8:11:74:PRO:O     | 8:11:77:VAL:HG22  | 2.14                     | 0.47              |
| 30:33:33:THR:HG23 | 30:33:34:LYS:H    | 1.79                     | 0.47              |
| 32:B:125:PHE:CE1  | 32:B:136:ARG:HB2  | 2.49                     | 0.47              |
| 33:C:39:ARG:NH1   | 33:C:54:ILE:CG1   | 2.74                     | 0.47              |
| 34:D:28:ASP:C     | 34:D:30:LYS:H     | 2.22                     | 0.47              |
| 34:D:43:ARG:HG2   | 34:D:43:ARG:HH11  | 1.78                     | 0.47              |
| 35:E:93:VAL:HG13  | 35:E:110:MET:CE   | 2.36                     | 0.47              |
| 37:G:25:PHE:HA    | 37:G:28:ILE:HD12  | 1.97                     | 0.47              |
| 37:G:108:ARG:HD3  | 37:G:115:MET:HE1  | 1.96                     | 0.47              |
| 41:K:28:ASN:OD1   | 41:K:46:ALA:HB3   | 2.14                     | 0.47              |
| 41:K:67:GLU:O     | 41:K:70:ALA:HB3   | 2.13                     | 0.47              |
| 41:K:91:GLY:O     | 41:K:92:ARG:C     | 2.57                     | 0.47              |
| 42:L:89:LEU:HD12  | 42:L:89:LEU:N     | 2.29                     | 0.47              |
| 43:M:27:THR:HG21  | 53:A:1328:C:OP1   | 2.14                     | 0.47              |
| 46:P:7:ALA:O      | 46:P:17:TYR:HA    | 2.14                     | 0.47              |
| 46:P:35:ARG:HH11  | 46:P:35:ARG:HG3   | 1.79                     | 0.47              |
| 53:A:424:G:O2'    | 53:A:425:G:H5'    | 2.13                     | 0.47              |
| 53:A:1394:A:H3'   | 53:A:1395:C:H5'   | 1.96                     | 0.47              |
| 53:A:1437:A:H2'   | 53:A:1438:G:H8    | 1.79                     | 0.47              |
| 54:01:596:U:H2'   | 54:01:597:G:C8    | 2.49                     | 0.47              |
| 54:01:1020:A:C1'  | 54:01:1021:A:OP2  | 2.55                     | 0.47              |
| 54:01:1097:U:H2'  | 54:01:1098:A:O4'  | 2.14                     | 0.47              |
| 54:01:2673:G:H2'  | 54:01:2674:G:H8   | 1.77                     | 0.47              |
| 7:10:56:ARG:HD2   | 54:01:1084:A:N3   | 2.30                     | 0.47              |
| 7:10:96:PHE:HE2   | 7:10:126:LEU:HB2  | 1.79                     | 0.47              |
| 8:11:74:PRO:O     | 8:11:78:LEU:HG    | 2.14                     | 0.47              |
| 10:13:17:ARG:HG2  | 10:13:17:ARG:HH11 | 1.79                     | 0.47              |
| 10:13:29:HIS:O    | 10:13:29:HIS:ND1  | 2.45                     | 0.47              |
| 10:13:58:LEU:O    | 10:13:58:LEU:HD12 | 2.15                     | 0.47              |
| 17:20:24:LYS:HA   | 17:20:94:THR:OG1  | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:22:50:LEU:HD12 | 19:22:50:LEU:N    | 2.29                     | 0.47              |
| 33:C:79:LYS:HG3   | 33:C:79:LYS:O     | 2.14                     | 0.47              |
| 49:S:9:PHE:O      | 49:S:10:ILE:HG23  | 2.13                     | 0.47              |
| 51:U:24:LYS:CG    | 51:U:25:ALA:N     | 2.73                     | 0.47              |
| 52:03:220:ALA:HA  | 54:01:2176:A:C5'  | 2.44                     | 0.47              |
| 53:A:1501:C:H5''  | 53:A:1502:A:OP2   | 2.14                     | 0.47              |
| 54:01:863:A:H2'   | 54:01:864:G:C8    | 2.49                     | 0.47              |
| 54:01:1775:U:C2'  | 54:01:1776:G:H5'  | 2.44                     | 0.47              |
| 54:01:1972:G:H2'  | 54:01:1973:G:C8   | 2.46                     | 0.47              |
| 54:01:2120:G:H2'  | 54:01:2121:G:C8   | 2.49                     | 0.47              |
| 54:01:2297:A:N1   | 54:01:2321:U:H5   | 2.12                     | 0.47              |
| 55:02:65:U:H3'    | 55:02:108:A:N6    | 2.24                     | 0.47              |
| 59:Z:49:PRO:HD2   | 59:Z:90:LYS:HE2   | 1.96                     | 0.47              |
| 1:04:215:VAL:HG12 | 1:04:216:ARG:N    | 2.29                     | 0.47              |
| 2:05:25:THR:HG21  | 2:05:193:VAL:HG22 | 1.95                     | 0.47              |
| 3:06:23:PHE:H     | 3:06:114:ARG:HH22 | 1.63                     | 0.47              |
| 3:06:83:VAL:O     | 3:06:84:THR:C     | 2.56                     | 0.47              |
| 6:09:7:ASP:CG     | 6:09:8:LYS:H      | 2.23                     | 0.47              |
| 6:09:45:GLU:HA    | 6:09:48:GLU:HG2   | 1.95                     | 0.47              |
| 14:17:2:ASP:N     | 14:17:5:SER:HG    | 2.11                     | 0.47              |
| 14:17:56:LYS:HA   | 14:17:59:ALA:HB3  | 1.95                     | 0.47              |
| 14:17:94:ARG:O    | 14:17:97:PHE:N    | 2.47                     | 0.47              |
| 18:21:33:LEU:CD2  | 18:21:51:LEU:HD23 | 2.44                     | 0.47              |
| 41:K:122:PRO:HG2  | 51:U:35:GLU:HA    | 1.96                     | 0.47              |
| 42:L:47:ALA:O     | 42:L:48:LEU:HD12  | 2.15                     | 0.47              |
| 46:P:54:LEU:CD1   | 46:P:80:LYS:HA    | 2.45                     | 0.47              |
| 50:T:34:VAL:O     | 50:T:38:ILE:HG13  | 2.15                     | 0.47              |
| 52:03:30:LEU:HD12 | 52:03:30:LEU:C    | 2.39                     | 0.47              |
| 53:A:24:U:H2'     | 53:A:25:C:C6      | 2.49                     | 0.47              |
| 53:A:123:U:H5''   | 53:A:311:C:O2'    | 2.15                     | 0.47              |
| 53:A:1123:U:O2'   | 53:A:1124:G:H5'   | 2.15                     | 0.47              |
| 54:01:145:C:H2'   | 54:01:146:A:H8    | 1.79                     | 0.47              |
| 54:01:2197:U:O2'  | 54:01:2198:A:H5'' | 2.14                     | 0.47              |
| 3:06:181:ILE:HG23 | 11:14:2:ARG:HG3   | 1.95                     | 0.47              |
| 4:07:176:PHE:O    | 4:07:177:ARG:C    | 2.57                     | 0.47              |
| 8:11:106:GLN:O    | 8:11:109:ALA:HB3  | 2.14                     | 0.47              |
| 13:16:78:LYS:HG3  | 13:16:82:GLU:OE1  | 2.15                     | 0.47              |
| 18:21:43:ALA:HA   | 18:21:46:LEU:HB2  | 1.95                     | 0.47              |
| 26:29:65:ASN:O    | 26:29:66:ILE:CB   | 2.58                     | 0.47              |
| 30:33:2:LYS:HG3   | 54:01:242:G:C8    | 2.50                     | 0.47              |
| 34:D:56:GLU:OE1   | 34:D:198:LEU:HD12 | 2.14                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:H:4:ASP:HB2     | 38:H:80:PRO:HG3    | 1.97                     | 0.47              |
| 41:K:30:ILE:HG23   | 41:K:30:ILE:O      | 2.15                     | 0.47              |
| 44:N:2:LYS:O       | 44:N:4:SER:N       | 2.47                     | 0.47              |
| 48:R:32:ILE:HG22   | 48:R:38:ILE:HA     | 1.96                     | 0.47              |
| 53:A:543:U:H2'     | 53:A:544:G:H8      | 1.78                     | 0.47              |
| 54:01:813:U:H2'    | 54:01:814:C:C6     | 2.49                     | 0.47              |
| 54:01:862:G:H2'    | 54:01:863:A:O4'    | 2.13                     | 0.47              |
| 54:01:980:A:N7     | 54:01:981:A:C6     | 2.83                     | 0.47              |
| 54:01:1788:C:O2'   | 54:01:1789:A:H5'   | 2.15                     | 0.47              |
| 54:01:2036:C:H2'   | 54:01:2037:A:H8    | 1.79                     | 0.47              |
| 54:01:2828:G:H2'   | 54:01:2829:A:H8    | 1.79                     | 0.47              |
| 1:04:259:ASN:O     | 1:04:260:LYS:HB2   | 2.14                     | 0.47              |
| 2:05:86:GLU:HG3    | 2:05:86:GLU:O      | 2.14                     | 0.47              |
| 5:08:132:LEU:HD12  | 5:08:132:LEU:C     | 2.39                     | 0.47              |
| 6:09:14:SER:OG     | 6:09:17:ASP:HB2    | 2.14                     | 0.47              |
| 7:10:3:LEU:HD12    | 7:10:3:LEU:C       | 2.40                     | 0.47              |
| 11:14:118:THR:O    | 11:14:120:VAL:HG23 | 2.14                     | 0.47              |
| 12:15:62:LYS:HD2   | 12:15:64:TRP:CZ2   | 2.50                     | 0.47              |
| 19:22:48:GLN:OE1   | 19:22:53:VAL:O     | 2.32                     | 0.47              |
| 20:23:96:LYS:C     | 20:23:98:ASN:N     | 2.68                     | 0.47              |
| 26:29:16:CYS:SG    | 26:29:18:CYS:HB2   | 2.54                     | 0.47              |
| 35:E:89:THR:HG22   | 35:E:90:GLY:N      | 2.29                     | 0.47              |
| 40:J:76:ILE:CD1    | 40:J:87:LEU:HD11   | 2.44                     | 0.47              |
| 43:M:89:ARG:HH21   | 43:M:95:PRO:HG2    | 1.79                     | 0.47              |
| 43:M:97:ARG:HH11   | 43:M:97:ARG:HG3    | 1.79                     | 0.47              |
| 44:N:29:ILE:O      | 44:N:32:ASP:OD2    | 2.32                     | 0.47              |
| 50:T:4:LYS:HG3     | 53:A:332:G:OP1     | 2.15                     | 0.47              |
| 52:03:217:THR:HG23 | 54:01:2124:G:H21   | 1.78                     | 0.47              |
| 53:A:955:U:H3      | 53:A:1225:A:H61    | 1.63                     | 0.47              |
| 53:A:1228:C:H2'    | 53:A:1229:A:H8     | 1.80                     | 0.47              |
| 54:01:290:U:H2'    | 54:01:291:G:C8     | 2.50                     | 0.47              |
| 54:01:2155:U:H2'   | 54:01:2156:G:H5'   | 1.96                     | 0.47              |
| 54:01:2572:A:OP1   | 54:01:2574:G:H4'   | 2.15                     | 0.47              |
| 54:01:2606:C:H2'   | 54:01:2607:G:H8    | 1.79                     | 0.47              |
| 2:05:158:GLY:HA3   | 9:12:80:HIS:HE2    | 1.79                     | 0.47              |
| 3:06:147:LEU:HD13  | 3:06:168:ASP:HB3   | 1.96                     | 0.47              |
| 5:08:44:HIS:CD2    | 5:08:45:ALA:H      | 2.32                     | 0.47              |
| 7:10:33:VAL:HG22   | 7:10:36:ASP:OD2    | 2.15                     | 0.47              |
| 8:11:61:TYR:C      | 8:11:63:ASP:H      | 2.22                     | 0.47              |
| 11:14:14:LYS:O     | 11:14:14:LYS:HG3   | 2.14                     | 0.47              |
| 12:15:3:GLN:HE21   | 12:15:92:TRP:NE1   | 2.11                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:17:27:VAL:HG13  | 14:17:95:SER:OG   | 2.15                     | 0.47              |
| 14:17:106:LEU:HD23 | 14:17:106:LEU:C   | 2.38                     | 0.47              |
| 15:18:52:ARG:NH2   | 54:01:2720:U:H5'' | 2.29                     | 0.47              |
| 15:18:90:ALA:CB    | 15:18:112:ARG:HB2 | 2.44                     | 0.47              |
| 16:19:50:ARG:HG3   | 16:19:50:ARG:NH1  | 2.26                     | 0.47              |
| 19:22:69:ARG:HG3   | 19:22:74:ILE:HG22 | 1.96                     | 0.47              |
| 29:32:25:LYS:HA    | 29:32:28:ARG:CZ   | 2.45                     | 0.47              |
| 32:B:208:ALA:O     | 32:B:211:LEU:HB3  | 2.15                     | 0.47              |
| 33:C:108:PRO:HA    | 33:C:114:LEU:HD12 | 1.95                     | 0.47              |
| 34:D:10:LEU:HD22   | 34:D:62:ARG:NH1   | 2.30                     | 0.47              |
| 39:I:91:GLU:C      | 39:I:93:LEU:H     | 2.20                     | 0.47              |
| 40:J:8:ILE:HG12    | 40:J:100:ILE:HG22 | 1.97                     | 0.47              |
| 42:L:49:ARG:HH22   | 53:A:522:C:H41    | 1.62                     | 0.47              |
| 43:M:16:ILE:H      | 43:M:16:ILE:CD1   | 2.26                     | 0.47              |
| 44:N:2:LYS:O       | 44:N:3:GLN:C      | 2.57                     | 0.47              |
| 46:P:22:ALA:HA     | 46:P:33:ILE:CD1   | 2.44                     | 0.47              |
| 48:R:12:PHE:C      | 48:R:14:ALA:N     | 2.69                     | 0.47              |
| 51:U:33:ARG:NH1    | 51:U:34:ARG:HG2   | 2.30                     | 0.47              |
| 52:03:15:VAL:HG13  | 52:03:21:TYR:CE2  | 2.49                     | 0.47              |
| 53:A:411:A:N9      | 53:A:413:G:H1'    | 2.30                     | 0.47              |
| 54:01:46:G:H2'     | 54:01:47:C:C6     | 2.50                     | 0.47              |
| 54:01:274:C:H2'    | 54:01:275:C:O4'   | 2.15                     | 0.47              |
| 54:01:1373:A:H2'   | 54:01:1374:G:O4'  | 2.15                     | 0.47              |
| 54:01:1564:C:H2'   | 54:01:1565:C:O4'  | 2.14                     | 0.47              |
| 54:01:2230:G:H2'   | 54:01:2231:U:C6   | 2.50                     | 0.47              |
| 54:01:2416:C:H2'   | 54:01:2417:C:C6   | 2.50                     | 0.47              |
| 54:01:2715:C:H2'   | 54:01:2716:C:O4'  | 2.15                     | 0.47              |
| 58:Y:61:C:H6       | 58:Y:61:C:H5'     | 1.80                     | 0.47              |
| 59:Z:32:ASP:O      | 59:Z:33:LYS:C     | 2.57                     | 0.47              |
| 7:10:48:ALA:HB1    | 7:10:51:TYR:OH    | 2.15                     | 0.47              |
| 11:14:51:GLU:O     | 54:01:833:A:H1'   | 2.15                     | 0.47              |
| 12:15:6:ARG:HG3    | 12:15:6:ARG:O     | 2.14                     | 0.47              |
| 12:15:59:ARG:HG3   | 12:15:59:ARG:NH2  | 2.30                     | 0.47              |
| 19:22:6:ARG:HH12   | 19:22:10:VAL:HG22 | 1.80                     | 0.47              |
| 19:22:59:ASN:HB2   | 19:22:84:TYR:HB2  | 1.96                     | 0.47              |
| 24:27:16:THR:O     | 24:27:19:LEU:HB2  | 2.15                     | 0.47              |
| 33:C:66:THR:HA     | 33:C:101:ASN:O    | 2.14                     | 0.47              |
| 35:E:63:MET:O      | 35:E:67:ARG:HG2   | 2.15                     | 0.47              |
| 35:E:111:ARG:HG3   | 35:E:111:ARG:NH1  | 2.28                     | 0.47              |
| 37:G:4:ARG:HB3     | 37:G:6:ILE:HG13   | 1.97                     | 0.47              |
| 48:R:16:GLY:O      | 48:R:18:GLN:HG2   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:R:48:ALA:O     | 48:R:51:GLN:HB3   | 2.15                     | 0.47              |
| 53:A:665:A:H1'    | 53:A:733:G:H1'    | 1.96                     | 0.47              |
| 53:A:744:C:H2'    | 53:A:745:G:C8     | 2.50                     | 0.47              |
| 53:A:1330:U:H2'   | 53:A:1331:G:O4'   | 2.15                     | 0.47              |
| 53:A:1356:G:H2'   | 53:A:1357:A:C8    | 2.49                     | 0.47              |
| 54:01:832:U:H2'   | 54:01:833:A:H8    | 1.80                     | 0.47              |
| 54:01:1268:A:H2'  | 54:01:1269:A:O4'  | 2.14                     | 0.47              |
| 54:01:1352:U:O2'  | 54:01:1353:A:H5'  | 2.14                     | 0.47              |
| 54:01:1435:G:H2'  | 54:01:1436:G:H8   | 1.80                     | 0.47              |
| 54:01:1771:C:N4   | 54:01:1772:A:N6   | 2.63                     | 0.47              |
| 54:01:2065:C:H2'  | 54:01:2066:C:C6   | 2.50                     | 0.47              |
| 54:01:2270:A:H2'  | 54:01:2271:G:O4'  | 2.15                     | 0.47              |
| 54:01:2591:C:H2'  | 54:01:2592:G:H8   | 1.79                     | 0.47              |
| 54:01:2732:G:O2'  | 54:01:2733:A:H5'  | 2.15                     | 0.47              |
| 56:X:71:C:H2'     | 56:X:72:A:H8      | 1.79                     | 0.47              |
| 59:Z:110:GLY:HA3  | 59:Z:124:LEU:CD2  | 2.42                     | 0.47              |
| 59:Z:133:GLY:HA2  | 59:Z:136:VAL:HB   | 1.96                     | 0.47              |
| 1:04:14:HIS:O     | 1:04:203:VAL:HG21 | 2.15                     | 0.47              |
| 1:04:18:VAL:CG2   | 1:04:202:ARG:HB2  | 2.45                     | 0.47              |
| 4:07:102:LEU:HA   | 4:07:106:ALA:CB   | 2.45                     | 0.47              |
| 6:09:63:ALA:HA    | 6:09:66:ASN:ND2   | 2.20                     | 0.47              |
| 6:09:85:GLY:N     | 6:09:91:PHE:HB2   | 2.30                     | 0.47              |
| 12:15:66:ARG:HB2  | 12:15:101:VAL:O   | 2.15                     | 0.47              |
| 14:17:49:VAL:HG11 | 14:17:81:ARG:HG3  | 1.97                     | 0.47              |
| 14:17:94:ARG:HB3  | 14:17:94:ARG:HH21 | 1.79                     | 0.47              |
| 18:21:40:ASN:C    | 18:21:41:LYS:HG2  | 2.40                     | 0.47              |
| 22:25:26:SER:HA   | 22:25:61:GLY:O    | 2.14                     | 0.47              |
| 32:B:22:TRP:CE3   | 32:B:30:ILE:HD11  | 2.49                     | 0.47              |
| 34:D:23:GLY:HA3   | 53:A:409:U:OP1    | 2.15                     | 0.47              |
| 36:F:32:ALA:HB2   | 36:F:70:VAL:HG21  | 1.97                     | 0.47              |
| 39:I:87:MET:HG3   | 39:I:88:GLU:H     | 1.80                     | 0.47              |
| 40:J:32:THR:HG23  | 40:J:32:THR:O     | 2.15                     | 0.47              |
| 48:R:12:PHE:O     | 48:R:14:ALA:N     | 2.48                     | 0.47              |
| 51:U:24:LYS:CG    | 51:U:25:ALA:H     | 2.28                     | 0.47              |
| 53:A:784:A:H2'    | 53:A:785:G:C8     | 2.49                     | 0.47              |
| 53:A:1402:C:H2'   | 53:A:1403:C:O4'   | 2.15                     | 0.47              |
| 53:A:1404:C:H2'   | 53:A:1405:G:C8    | 2.50                     | 0.47              |
| 53:A:1477:U:H2'   | 53:A:1478:U:C6    | 2.50                     | 0.47              |
| 54:01:290:U:H2'   | 54:01:291:G:H8    | 1.80                     | 0.47              |
| 54:01:622:G:H2'   | 54:01:623:C:C6    | 2.50                     | 0.47              |
| 54:01:2371:G:HO2' | 54:01:2372:U:H5'  | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:05:77:ARG:NH2   | 2:05:200:ASP:OD1  | 2.48                     | 0.47              |
| 2:05:98:VAL:HG23  | 2:05:101:PHE:HD2  | 1.80                     | 0.47              |
| 3:06:115:GLN:HB3  | 3:06:117:ARG:HG3  | 1.96                     | 0.47              |
| 4:07:102:LEU:O    | 4:07:106:ALA:HB3  | 2.15                     | 0.47              |
| 5:08:102:ILE:HD11 | 5:08:116:LEU:HD21 | 1.96                     | 0.47              |
| 6:09:42:LYS:HB3   | 6:09:46:PHE:CE2   | 2.50                     | 0.47              |
| 6:09:77:THR:HA    | 6:09:143:ILE:O    | 2.14                     | 0.47              |
| 9:12:4:PHE:CG     | 16:19:99:VAL:HG11 | 2.49                     | 0.47              |
| 9:12:40:HIS:NE2   | 9:12:52:ASP:OD2   | 2.44                     | 0.47              |
| 9:12:49:ASP:HB2   | 9:12:118:MET:HE2  | 1.97                     | 0.47              |
| 15:18:38:ARG:HD2  | 53:A:345:C:OP1    | 2.14                     | 0.47              |
| 15:18:91:VAL:HG21 | 15:18:96:LEU:HD21 | 1.96                     | 0.47              |
| 32:B:215:ALA:O    | 32:B:218:ALA:HB3  | 2.15                     | 0.47              |
| 37:G:68:VAL:O     | 37:G:70:PRO:HD3   | 2.15                     | 0.47              |
| 39:I:104:THR:HG22 | 39:I:106:ASP:N    | 2.10                     | 0.47              |
| 40:J:9:ARG:HH12   | 40:J:11:LYS:CE    | 2.28                     | 0.47              |
| 41:K:108:ASN:HB3  | 51:U:6:ARG:HG3    | 1.96                     | 0.47              |
| 42:L:98:ARG:HD2   | 42:L:103:CYS:SG   | 2.55                     | 0.47              |
| 53:A:401:C:H2'    | 53:A:402:G:H8     | 1.80                     | 0.47              |
| 53:A:631:C:H3'    | 53:A:632:U:H5'    | 1.96                     | 0.47              |
| 53:A:1195:C:H5''  | 53:A:1196:A:OP2   | 2.14                     | 0.47              |
| 54:01:940:G:H2'   | 54:01:941:A:H5''  | 1.96                     | 0.47              |
| 54:01:1344:U:H3'  | 54:01:1345:C:H5'  | 1.96                     | 0.47              |
| 54:01:1802:A:H2'  | 54:01:1803:A:C8   | 2.50                     | 0.47              |
| 54:01:2208:C:H2'  | 54:01:2209:G:H8   | 1.80                     | 0.47              |
| 54:01:2472:G:H2'  | 54:01:2475:C:H42  | 1.80                     | 0.47              |
| 54:01:2884:U:O2   | 54:01:2884:U:H3'  | 2.14                     | 0.47              |
| 2:05:77:ARG:HG3   | 2:05:77:ARG:O     | 2.15                     | 0.46              |
| 4:07:94:ARG:O     | 4:07:97:GLU:HB3   | 2.15                     | 0.46              |
| 8:11:52:LEU:HD12  | 8:11:52:LEU:N     | 2.29                     | 0.46              |
| 11:14:111:ILE:CG2 | 11:14:112:LEU:N   | 2.78                     | 0.46              |
| 13:16:63:ARG:HD3  | 54:01:1454:C:O4'  | 2.15                     | 0.46              |
| 16:19:29:ARG:HH12 | 27:30:9:ARG:NE    | 2.13                     | 0.46              |
| 28:31:32:LYS:HD2  | 28:31:50:GLU:HB3  | 1.97                     | 0.46              |
| 40:J:86:ALA:O     | 40:J:90:LEU:HD12  | 2.16                     | 0.46              |
| 41:K:66:ALA:O     | 41:K:70:ALA:N     | 2.47                     | 0.46              |
| 42:L:87:LYS:HG2   | 42:L:87:LYS:O     | 2.14                     | 0.46              |
| 53:A:434:U:H2'    | 53:A:435:A:C8     | 2.50                     | 0.46              |
| 53:A:922:G:H2'    | 53:A:923:A:C8     | 2.50                     | 0.46              |
| 54:01:662:G:H2'   | 54:01:663:G:H8    | 1.79                     | 0.46              |
| 54:01:680:C:H2'   | 54:01:681:G:H8    | 1.79                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:01:1903:G:H2'  | 54:01:1904:G:H8   | 1.79                     | 0.46              |
| 54:01:2066:C:O2'  | 54:01:2067:G:H5'  | 2.15                     | 0.46              |
| 54:01:2215:C:H2'  | 54:01:2216:G:H8   | 1.80                     | 0.46              |
| 54:01:2860:A:H2'  | 54:01:2861:U:H5'  | 1.97                     | 0.46              |
| 1:04:19:VAL:HG21  | 54:01:1565:C:OP1  | 2.15                     | 0.46              |
| 1:04:115:ILE:O    | 1:04:116:GLN:HB3  | 2.15                     | 0.46              |
| 8:11:24:GLY:O     | 8:11:27:LEU:HG    | 2.15                     | 0.46              |
| 12:15:55:ARG:CD   | 54:01:2469:A:H4'  | 2.45                     | 0.46              |
| 16:19:48:ASP:HA   | 16:19:51:GLN:HB2  | 1.98                     | 0.46              |
| 18:21:6:LYS:CG    | 54:01:494:G:H4'   | 2.43                     | 0.46              |
| 32:B:202:ASN:ND2  | 32:B:205:ALA:HB3  | 2.29                     | 0.46              |
| 34:D:8:LEU:HD21   | 34:D:31:CYS:CB    | 2.45                     | 0.46              |
| 35:E:98:ALA:CB    | 35:E:123:LEU:HG   | 2.45                     | 0.46              |
| 38:H:12:ARG:HD3   | 38:H:26:MET:HB3   | 1.95                     | 0.46              |
| 39:I:114:LYS:HB2  | 39:I:117:LEU:HD22 | 1.96                     | 0.46              |
| 40:J:53:ILE:HG13  | 44:N:84:ARG:CD    | 2.45                     | 0.46              |
| 44:N:60:ARG:O     | 44:N:61:ASN:HB2   | 2.16                     | 0.46              |
| 50:T:70:LYS:HG3   | 50:T:73:ARG:HH22  | 1.81                     | 0.46              |
| 53:A:695:A:H2'    | 53:A:696:A:C8     | 2.51                     | 0.46              |
| 54:01:871:U:H2'   | 54:01:872:U:C6    | 2.50                     | 0.46              |
| 54:01:1196:C:H2'  | 54:01:1197:G:C8   | 2.50                     | 0.46              |
| 54:01:1363:C:H2'  | 54:01:1364:G:H8   | 1.80                     | 0.46              |
| 54:01:1642:G:O2'  | 54:01:1643:G:H5'  | 2.15                     | 0.46              |
| 54:01:2001:C:H1'  | 54:01:2689:U:C4   | 2.50                     | 0.46              |
| 54:01:2646:C:H2'  | 54:01:2647:U:O4'  | 2.15                     | 0.46              |
| 2:05:90:PHE:HD1   | 2:05:94:GLN:NE2   | 2.13                     | 0.46              |
| 4:07:70:ARG:NH2   | 4:07:71:LYS:HG2   | 2.31                     | 0.46              |
| 5:08:100:ASN:CA   | 5:08:116:LEU:HD12 | 2.45                     | 0.46              |
| 6:09:3:VAL:HG13   | 6:09:37:VAL:O     | 2.15                     | 0.46              |
| 8:11:62:ALA:C     | 8:11:64:ARG:H     | 2.22                     | 0.46              |
| 9:12:77:HIS:ND1   | 9:12:79:GLY:N     | 2.59                     | 0.46              |
| 10:13:79:PHE:CD1  | 15:18:69:VAL:HG22 | 2.48                     | 0.46              |
| 15:18:38:ARG:HH21 | 15:18:38:ARG:HG3  | 1.80                     | 0.46              |
| 18:21:18:ARG:CZ   | 54:01:518:G:H4'   | 2.45                     | 0.46              |
| 30:33:3:ILE:HG22  | 30:33:4:LYS:O     | 2.16                     | 0.46              |
| 32:B:109:SER:O    | 32:B:112:ARG:HB3  | 2.15                     | 0.46              |
| 39:I:30:ASN:ND2   | 39:I:65:THR:HA    | 2.29                     | 0.46              |
| 40:J:41:PRO:O     | 40:J:42:LEU:HB2   | 2.13                     | 0.46              |
| 44:N:2:LYS:O      | 44:N:5:MET:N      | 2.48                     | 0.46              |
| 46:P:8:ARG:O      | 46:P:9:HIS:ND1    | 2.48                     | 0.46              |
| 53:A:62:U:O2'     | 53:A:379:C:H1'    | 2.16                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:A:285:C:H2'    | 53:A:286:C:C6      | 2.49                     | 0.46              |
| 53:A:1032:G:H3'   | 53:A:1032:G:N3     | 2.31                     | 0.46              |
| 53:A:1163:A:H2'   | 53:A:1164:G:C8     | 2.50                     | 0.46              |
| 53:A:1201:A:C1'   | 53:A:1202:U:OP2    | 2.57                     | 0.46              |
| 54:01:848:C:H2'   | 54:01:849:A:C8     | 2.50                     | 0.46              |
| 54:01:1060:U:C5'  | 54:01:1062:G:H5'   | 2.44                     | 0.46              |
| 54:01:1209:U:H2'  | 54:01:1210:G:H21   | 1.80                     | 0.46              |
| 54:01:1637:A:H2'  | 54:01:1638:C:C6    | 2.51                     | 0.46              |
| 54:01:2443:C:H2'  | 54:01:2444:G:C8    | 2.49                     | 0.46              |
| 1:04:116:GLN:HG3  | 1:04:121:ALA:HB2   | 1.97                     | 0.46              |
| 3:06:109:LEU:HD11 | 3:06:180:LEU:HD13  | 1.97                     | 0.46              |
| 3:06:117:ARG:HH12 | 11:14:2:ARG:CB     | 2.27                     | 0.46              |
| 4:07:66:ILE:HG12  | 55:02:41:G:H22     | 1.80                     | 0.46              |
| 5:08:23:ILE:HG21  | 5:08:71:LEU:HD21   | 1.97                     | 0.46              |
| 7:10:107:GLU:O    | 7:10:108:VAL:HB    | 2.16                     | 0.46              |
| 13:16:94:TYR:O    | 13:16:116:VAL:HG23 | 2.16                     | 0.46              |
| 16:19:47:ARG:HG3  | 54:01:1156:A:N6    | 2.30                     | 0.46              |
| 17:20:38:VAL:O    | 17:20:38:VAL:HG13  | 2.14                     | 0.46              |
| 21:24:60:VAL:HG22 | 21:24:73:LYS:HE3   | 1.98                     | 0.46              |
| 26:29:2:LYS:HB2   | 26:29:5:ILE:HD13   | 1.96                     | 0.46              |
| 27:30:14:MET:SD   | 54:01:2045:C:H5''  | 2.55                     | 0.46              |
| 32:B:41:ASN:HA    | 59:Z:5:PHE:CE2     | 2.50                     | 0.46              |
| 33:C:63:ILE:HG22  | 33:C:97:PRO:O      | 2.16                     | 0.46              |
| 34:D:36:ALA:H     | 34:D:37:PRO:CD     | 2.23                     | 0.46              |
| 34:D:49:ASP:O     | 34:D:52:VAL:HG22   | 2.15                     | 0.46              |
| 34:D:193:ASP:OD1  | 34:D:194:ILE:HG23  | 2.16                     | 0.46              |
| 35:E:76:ASN:O     | 35:E:79:THR:HG22   | 2.16                     | 0.46              |
| 37:G:35:LYS:O     | 37:G:38:ALA:HB3    | 2.16                     | 0.46              |
| 38:H:95:MET:O     | 38:H:97:GLY:N      | 2.48                     | 0.46              |
| 40:J:5:ARG:N      | 40:J:77:VAL:O      | 2.49                     | 0.46              |
| 43:M:2:ARG:HE     | 43:M:8:ILE:CD1     | 2.16                     | 0.46              |
| 44:N:25:GLU:O     | 44:N:29:ILE:N      | 2.48                     | 0.46              |
| 49:S:9:PHE:HE2    | 49:S:36:ARG:HE     | 1.64                     | 0.46              |
| 49:S:65:MET:HG2   | 49:S:73:PHE:CZ     | 2.51                     | 0.46              |
| 53:A:1316:G:H2'   | 53:A:1317:C:H5''   | 1.97                     | 0.46              |
| 54:01:1355:G:H2'  | 54:01:1356:G:H8    | 1.81                     | 0.46              |
| 54:01:2053:G:O2'  | 54:01:2054:A:H5'   | 2.14                     | 0.46              |
| 54:01:2609:U:H5'  | 54:01:2610:C:OP2   | 2.14                     | 0.46              |
| 7:10:56:ARG:HH21  | 7:10:83:ALA:HB2    | 1.78                     | 0.46              |
| 9:12:27:ARG:NH2   | 54:01:1142:A:H4'   | 2.31                     | 0.46              |
| 9:12:98:GLU:OE2   | 9:12:125:TYR:HA    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:14:61:LEU:O    | 30:33:12:ARG:HD3  | 2.16                     | 0.46              |
| 18:21:69:LEU:HG   | 18:21:107:VAL:CG2 | 2.46                     | 0.46              |
| 22:25:64:LYS:HB2  | 22:25:79:GLU:OE1  | 2.15                     | 0.46              |
| 27:30:56:LYS:OXT  | 27:30:56:LYS:HG2  | 2.15                     | 0.46              |
| 29:32:3:ARG:HD2   | 29:32:4:THR:H     | 1.80                     | 0.46              |
| 31:34:25:VAL:HB   | 31:34:35:GLN:HG3  | 1.97                     | 0.46              |
| 41:K:117:HIS:O    | 41:K:118:ASN:HB2  | 2.15                     | 0.46              |
| 42:L:34:THR:O     | 42:L:53:ARG:HB3   | 2.14                     | 0.46              |
| 46:P:69:ASP:CG    | 46:P:70:ARG:H     | 2.23                     | 0.46              |
| 50:T:20:ASN:HD22  | 53:A:323:U:H5'    | 1.80                     | 0.46              |
| 51:U:56:ALA:O     | 51:U:59:LEU:HB3   | 2.16                     | 0.46              |
| 53:A:1198:G:H5'   | 53:A:1198:G:H8    | 1.81                     | 0.46              |
| 54:01:16:C:O2'    | 54:01:17:G:H5'    | 2.15                     | 0.46              |
| 54:01:27:G:H22    | 54:01:512:G:H1'   | 1.79                     | 0.46              |
| 54:01:140:C:H2'   | 54:01:141:G:H4'   | 1.97                     | 0.46              |
| 54:01:176:A:O2'   | 54:01:177:G:H5'   | 2.14                     | 0.46              |
| 54:01:1594:U:H2'  | 54:01:1595:C:C6   | 2.51                     | 0.46              |
| 54:01:2134:A:C6   | 54:01:2157:G:H4'  | 2.49                     | 0.46              |
| 55:02:88:C:C4'    | 55:02:89:U:OP1    | 2.63                     | 0.46              |
| 4:07:74:ALA:C     | 4:07:77:LYS:H     | 2.24                     | 0.46              |
| 5:08:67:ALA:O     | 5:08:70:LEU:HB2   | 2.16                     | 0.46              |
| 14:17:17:LYS:HZ1  | 54:01:2380:C:C5'  | 2.23                     | 0.46              |
| 34:D:7:LYS:HZ2    | 34:D:21:LYS:HG3   | 1.77                     | 0.46              |
| 39:I:81:GLY:O     | 39:I:85:ALA:N     | 2.49                     | 0.46              |
| 40:J:5:ARG:O      | 40:J:102:LEU:HA   | 2.15                     | 0.46              |
| 46:P:2:VAL:HG23   | 46:P:2:VAL:O      | 2.15                     | 0.46              |
| 47:Q:73:THR:HG22  | 47:Q:74:LEU:N     | 2.30                     | 0.46              |
| 53:A:10:A:H2'     | 53:A:11:G:C8      | 2.49                     | 0.46              |
| 53:A:337:G:H2'    | 53:A:338:A:C8     | 2.51                     | 0.46              |
| 53:A:1296:C:H4'   | 53:A:1302:C:N4    | 2.31                     | 0.46              |
| 54:01:558:U:H2'   | 54:01:559:G:H8    | 1.80                     | 0.46              |
| 54:01:1423:G:H2'  | 54:01:1424:G:H8   | 1.79                     | 0.46              |
| 54:01:1664:A:H61  | 54:01:1996:C:N4   | 1.99                     | 0.46              |
| 54:01:2682:A:O2'  | 54:01:2683:C:H5'  | 2.16                     | 0.46              |
| 55:02:2:G:H2'     | 55:02:3:C:C6      | 2.51                     | 0.46              |
| 2:05:77:ARG:HG3   | 2:05:77:ARG:NH2   | 2.30                     | 0.46              |
| 12:15:11:LYS:HD3  | 12:15:86:LYS:CG   | 2.45                     | 0.46              |
| 12:15:45:GLN:O    | 12:15:46:ILE:C    | 2.57                     | 0.46              |
| 14:17:31:THR:HG23 | 55:02:29:A:OP2    | 2.15                     | 0.46              |
| 14:17:79:ALA:O    | 14:17:83:LEU:HG   | 2.15                     | 0.46              |
| 16:19:19:GLN:HE22 | 17:20:73:LYS:HE2  | 1.80                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:21:43:ALA:HA   | 18:21:46:LEU:HD12  | 1.96                     | 0.46              |
| 18:21:50:VAL:O    | 18:21:53:SER:HB3   | 2.16                     | 0.46              |
| 19:22:54:GLU:OE1  | 19:22:54:GLU:N     | 2.48                     | 0.46              |
| 33:C:96:VAL:HB    | 33:C:97:PRO:CD     | 2.41                     | 0.46              |
| 34:D:144:ILE:HD13 | 34:D:177:MET:HB3   | 1.97                     | 0.46              |
| 35:E:122:VAL:HG23 | 35:E:122:VAL:O     | 2.16                     | 0.46              |
| 44:N:63:CYS:HB2   | 44:N:79:SER:HB2    | 1.98                     | 0.46              |
| 44:N:80:ARG:HA    | 44:N:83:VAL:HG12   | 1.98                     | 0.46              |
| 47:Q:39:ARG:HA    | 53:A:280:C:O2      | 2.16                     | 0.46              |
| 51:U:6:ARG:HH11   | 51:U:6:ARG:HB2     | 1.79                     | 0.46              |
| 53:A:497:G:H2'    | 53:A:498:A:C8      | 2.51                     | 0.46              |
| 53:A:1125:U:H2'   | 53:A:1126:U:H2'    | 1.98                     | 0.46              |
| 54:01:468:G:H2'   | 54:01:469:G:O4'    | 2.16                     | 0.46              |
| 54:01:656:G:O2'   | 54:01:657:U:H5'    | 2.16                     | 0.46              |
| 54:01:1047:G:H2'  | 54:01:1110:G:N2    | 2.31                     | 0.46              |
| 54:01:1396:U:H5'' | 54:01:1397:U:OP2   | 2.16                     | 0.46              |
| 54:01:2231:U:H2'  | 54:01:2232:C:C6    | 2.50                     | 0.46              |
| 54:01:2818:U:H2'  | 54:01:2819:G:C8    | 2.48                     | 0.46              |
| 1:04:48:ILE:O     | 1:04:48:ILE:HG23   | 2.15                     | 0.46              |
| 5:08:68:ARG:HG2   | 5:08:68:ARG:NH1    | 2.31                     | 0.46              |
| 6:09:16:GLY:HA2   | 6:09:47:PHE:CZ     | 2.50                     | 0.46              |
| 7:10:5:LEU:O      | 7:10:9:GLN:N       | 2.45                     | 0.46              |
| 7:10:34:THR:HG23  | 54:01:1056:G:H5'   | 1.98                     | 0.46              |
| 9:12:49:ASP:CG    | 9:12:118:MET:HB3   | 2.41                     | 0.46              |
| 11:14:95:LEU:HD11 | 11:14:125:LEU:HD21 | 1.97                     | 0.46              |
| 13:16:103:ARG:NH2 | 13:16:110:MET:HE3  | 2.31                     | 0.46              |
| 22:25:35:ARG:HH11 | 22:25:35:ARG:HG3   | 1.80                     | 0.46              |
| 24:27:1:MET:HE2   | 24:27:49:ASP:OD1   | 2.16                     | 0.46              |
| 25:28:12:ALA:HB2  | 25:28:23:LEU:CD1   | 2.46                     | 0.46              |
| 27:30:3:GLN:HA    | 54:01:2615:U:C2    | 2.50                     | 0.46              |
| 36:F:90:MET:HE3   | 48:R:60:ARG:NH1    | 2.31                     | 0.46              |
| 39:I:89:TYR:HB3   | 39:I:93:LEU:HD12   | 1.98                     | 0.46              |
| 48:R:21:ASP:OD2   | 48:R:23:LYS:HE2    | 2.15                     | 0.46              |
| 48:R:51:GLN:O     | 48:R:54:LEU:HB3    | 2.15                     | 0.46              |
| 51:U:37:TYR:CE2   | 53:A:1525:G:H5''   | 2.51                     | 0.46              |
| 53:A:948:C:H2'    | 53:A:949:A:H8      | 1.81                     | 0.46              |
| 54:01:43:G:H2'    | 54:01:44:A:O4'     | 2.16                     | 0.46              |
| 54:01:809:G:C5    | 54:01:810:U:C4     | 3.04                     | 0.46              |
| 54:01:1346:G:H2'  | 54:01:1347:A:C8    | 2.51                     | 0.46              |
| 54:01:1420:A:H5'  | 54:01:1421:G:OP2   | 2.16                     | 0.46              |
| 54:01:2442:C:O2'  | 54:01:2443:C:H5'   | 2.16                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 54:01:2489:U:C2'   | 54:01:2490:G:H5'  | 2.46                     | 0.46              |
| 54:01:2655:G:O2'   | 54:01:2656:U:H5   | 1.98                     | 0.46              |
| 54:01:2757:A:H2'   | 54:01:2757:A:N3   | 2.30                     | 0.46              |
| 55:02:39:A:H2'     | 55:02:40:U:C5     | 2.50                     | 0.46              |
| 1:04:252:LYS:NZ    | 54:01:1825:U:H1'  | 2.31                     | 0.46              |
| 4:07:67:THR:N      | 4:07:85:GLY:O     | 2.40                     | 0.46              |
| 4:07:174:PHE:O     | 4:07:176:PHE:N    | 2.49                     | 0.46              |
| 10:13:9:ASN:O      | 10:13:83:ALA:HA   | 2.16                     | 0.46              |
| 11:14:69:ARG:HH11  | 11:14:69:ARG:HG3  | 1.81                     | 0.46              |
| 33:C:49:ALA:HB1    | 33:C:75:VAL:HG22  | 1.98                     | 0.46              |
| 33:C:131:ARG:HE    | 33:C:135:ARG:NH2  | 2.06                     | 0.46              |
| 34:D:3:TYR:C       | 34:D:4:LEU:HG     | 2.41                     | 0.46              |
| 34:D:7:LYS:HZ1     | 34:D:21:LYS:HG3   | 1.80                     | 0.46              |
| 34:D:57:LYS:HD2    | 34:D:203:TYR:OH   | 2.15                     | 0.46              |
| 36:F:51:ILE:CG2    | 36:F:86:ARG:HE    | 2.29                     | 0.46              |
| 44:N:43:ALA:C      | 44:N:45:LEU:H     | 2.22                     | 0.46              |
| 45:O:71:ARG:NH2    | 53:A:754:C:H5'    | 2.31                     | 0.46              |
| 47:Q:57:VAL:HG12   | 47:Q:58:VAL:H     | 1.81                     | 0.46              |
| 53:A:86:G:H4'      | 53:A:87:C:C6      | 2.51                     | 0.46              |
| 54:01:7:G:H2'      | 54:01:8:C:C6      | 2.51                     | 0.46              |
| 54:01:207:A:H2'    | 54:01:208:C:O4'   | 2.16                     | 0.46              |
| 54:01:1188:U:O2'   | 54:01:1189:A:H5'  | 2.15                     | 0.46              |
| 54:01:1258:U:H2'   | 54:01:1259:G:C8   | 2.51                     | 0.46              |
| 54:01:1999:C:H2'   | 54:01:2000:C:C6   | 2.50                     | 0.46              |
| 54:01:2564:A:OP1   | 54:01:2648:G:H4'  | 2.15                     | 0.46              |
| 4:07:39:VAL:HG13   | 4:07:40:GLY:N     | 2.31                     | 0.46              |
| 7:10:55:VAL:HG23   | 7:10:84:TYR:HB2   | 1.97                     | 0.46              |
| 16:19:108:LEU:HD23 | 17:20:48:LYS:HZ3  | 1.81                     | 0.46              |
| 17:20:49:ILE:HD12  | 17:20:52:PRO:HA   | 1.98                     | 0.46              |
| 17:20:84:ARG:HB2   | 17:20:84:ARG:HH21 | 1.81                     | 0.46              |
| 21:24:82:TYR:CD1   | 21:24:83:LYS:HG3  | 2.51                     | 0.46              |
| 26:29:37:CYS:HG    | 26:29:40:CYS:HB3  | 1.80                     | 0.46              |
| 38:H:29:SER:O      | 38:H:33:VAL:HG23  | 2.16                     | 0.46              |
| 41:K:39:ASN:HD22   | 53:A:683:G:H21    | 1.64                     | 0.46              |
| 41:K:100:ASN:ND2   | 41:K:106:ILE:HG13 | 2.31                     | 0.46              |
| 43:M:66:GLY:O      | 43:M:67:ASP:C     | 2.58                     | 0.46              |
| 46:P:46:LYS:NZ     | 46:P:48:GLU:HB3   | 2.31                     | 0.46              |
| 53:A:86:G:H5''     | 53:A:87:C:OP1     | 2.16                     | 0.46              |
| 53:A:399:G:H2'     | 53:A:400:C:C6     | 2.51                     | 0.46              |
| 53:A:560:A:H4'     | 53:A:561:U:H5'    | 1.98                     | 0.46              |
| 53:A:709:U:H2'     | 53:A:710:G:C8     | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:A:763:G:H2'    | 53:A:764:C:C6     | 2.49                     | 0.46              |
| 53:A:815:A:H5''   | 53:A:817:C:N4     | 2.31                     | 0.46              |
| 53:A:860:A:H2'    | 53:A:861:G:O4'    | 2.17                     | 0.46              |
| 53:A:881:G:O2'    | 53:A:882:C:H5'    | 2.16                     | 0.46              |
| 53:A:882:C:O2'    | 53:A:883:C:H5'    | 2.15                     | 0.46              |
| 53:A:1325:C:O2'   | 53:A:1326:U:H5'   | 2.15                     | 0.46              |
| 53:A:1404:C:H2'   | 53:A:1405:G:H8    | 1.81                     | 0.46              |
| 54:01:783:A:H2'   | 54:01:784:G:H4'   | 1.98                     | 0.46              |
| 54:01:2631:G:O2'  | 54:01:2632:A:H5'  | 2.15                     | 0.46              |
| 54:01:2795:C:H2'  | 54:01:2796:U:O4'  | 2.16                     | 0.46              |
| 54:01:2798:U:H4'  | 54:01:2799:A:C4   | 2.51                     | 0.46              |
| 12:15:66:ARG:HG3  | 12:15:66:ARG:NH1  | 2.31                     | 0.45              |
| 23:26:63:ILE:HG23 | 23:26:64:ASP:N    | 2.31                     | 0.45              |
| 27:30:11:LYS:HA   | 27:30:14:MET:CE   | 2.46                     | 0.45              |
| 28:31:13:SER:OG   | 28:31:46:VAL:HG12 | 2.16                     | 0.45              |
| 32:B:131:LYS:O    | 32:B:135:MET:N    | 2.39                     | 0.45              |
| 32:B:202:ASN:CB   | 59:Z:43:LYS:HZ1   | 2.29                     | 0.45              |
| 36:F:49:TYR:CE1   | 36:F:51:ILE:HG12  | 2.51                     | 0.45              |
| 39:I:119:LYS:O    | 39:I:121:ARG:N    | 2.43                     | 0.45              |
| 39:I:122:ARG:NH1  | 39:I:123:ARG:O    | 2.49                     | 0.45              |
| 43:M:84:CYS:O     | 43:M:88:LEU:HD13  | 2.16                     | 0.45              |
| 47:Q:11:VAL:HG13  | 47:Q:20:ILE:HD11  | 1.97                     | 0.45              |
| 48:R:35:SER:O     | 48:R:70:THR:HA    | 2.16                     | 0.45              |
| 53:A:86:G:H4'     | 53:A:87:C:C5      | 2.51                     | 0.45              |
| 53:A:467:U:H5'    | 53:A:468:A:OP2    | 2.16                     | 0.45              |
| 53:A:918:A:H2'    | 53:A:919:A:O4'    | 2.16                     | 0.45              |
| 53:A:1484:C:H2'   | 53:A:1485:U:H6    | 1.79                     | 0.45              |
| 54:01:863:A:H2'   | 54:01:864:G:H8    | 1.81                     | 0.45              |
| 54:01:968:C:H2'   | 54:01:969:G:C8    | 2.51                     | 0.45              |
| 54:01:1190:G:H2'  | 54:01:1191:G:C8   | 2.50                     | 0.45              |
| 54:01:1430:G:H2'  | 54:01:1431:A:O4'  | 2.17                     | 0.45              |
| 54:01:2246:G:H2'  | 54:01:2247:A:C8   | 2.51                     | 0.45              |
| 54:01:2573:C:OP1  | 54:01:2574:G:H5'' | 2.16                     | 0.45              |
| 54:01:2638:G:H1'  | 54:01:2778:A:H61  | 1.81                     | 0.45              |
| 54:01:2699:C:O2'  | 54:01:2700:A:H5'  | 2.16                     | 0.45              |
| 54:01:2798:U:H4'  | 54:01:2799:A:C5   | 2.50                     | 0.45              |
| 1:04:175:LEU:HD12 | 1:04:179:GLU:HG2  | 1.99                     | 0.45              |
| 15:18:113:LEU:O   | 15:18:113:LEU:CD1 | 2.64                     | 0.45              |
| 20:23:13:LEU:HD11 | 20:23:70:ALA:HB2  | 1.98                     | 0.45              |
| 25:28:40:THR:HG23 | 25:28:43:ILE:H    | 1.81                     | 0.45              |
| 34:D:25:ARG:HH22  | 34:D:30:LYS:NZ    | 2.08                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:H:47:ASP:O     | 38:H:48:PHE:HB3   | 2.16                     | 0.45              |
| 40:J:17:LEU:O     | 40:J:20:GLN:HG2   | 2.15                     | 0.45              |
| 40:J:100:ILE:HD12 | 40:J:100:ILE:C    | 2.41                     | 0.45              |
| 41:K:90:PRO:HG2   | 41:K:91:GLY:H     | 1.81                     | 0.45              |
| 42:L:76:HIS:O     | 42:L:77:SER:OG    | 2.30                     | 0.45              |
| 43:M:100:ARG:HG3  | 53:A:950:U:OP2    | 2.15                     | 0.45              |
| 46:P:7:ALA:HB3    | 46:P:18:GLN:HB2   | 1.98                     | 0.45              |
| 53:A:152:A:H2'    | 53:A:153:C:H5'    | 1.98                     | 0.45              |
| 53:A:184:G:H4'    | 53:A:224:U:H4'    | 1.98                     | 0.45              |
| 53:A:273:U:H2'    | 53:A:274:A:H5'    | 1.97                     | 0.45              |
| 53:A:571:U:H4'    | 53:A:819:A:C6     | 2.51                     | 0.45              |
| 53:A:692:U:H2'    | 53:A:694:A:OP2    | 2.16                     | 0.45              |
| 53:A:1508:A:H2'   | 53:A:1509:C:C6    | 2.52                     | 0.45              |
| 54:01:214:G:O2'   | 54:01:215:G:H5'   | 2.16                     | 0.45              |
| 54:01:1279:G:H2'  | 54:01:1280:G:H8   | 1.81                     | 0.45              |
| 54:01:2087:G:H2'  | 54:01:2088:A:C8   | 2.52                     | 0.45              |
| 54:01:2318:G:H2'  | 54:01:2319:G:O4'  | 2.17                     | 0.45              |
| 55:02:49:C:H2'    | 55:02:50:A:C8     | 2.50                     | 0.45              |
| 59:Z:55:ASN:HD22  | 59:Z:61:GLU:HG3   | 1.80                     | 0.45              |
| 59:Z:157:ILE:HG23 | 59:Z:158:LYS:N    | 2.31                     | 0.45              |
| 1:04:42:ARG:O     | 54:01:1813:G:H4'  | 2.16                     | 0.45              |
| 1:04:224:MET:HG2  | 54:01:782:A:C2    | 2.51                     | 0.45              |
| 2:05:2:ILE:HD11   | 2:05:100:LEU:HD21 | 1.98                     | 0.45              |
| 9:12:27:ARG:HG3   | 9:12:27:ARG:NH1   | 2.31                     | 0.45              |
| 10:13:76:VAL:H    | 15:18:72:VAL:HG22 | 1.82                     | 0.45              |
| 13:16:73:ASN:O    | 13:16:74:GLU:C    | 2.59                     | 0.45              |
| 14:17:110:ALA:HB3 | 14:17:117:PHE:CE2 | 2.51                     | 0.45              |
| 23:26:18:SER:HB2  | 54:01:2080:A:H5'  | 1.97                     | 0.45              |
| 28:31:25:ASN:OD1  | 28:31:28:THR:HG23 | 2.16                     | 0.45              |
| 33:C:109:GLU:HB2  | 33:C:143:LEU:HD23 | 1.97                     | 0.45              |
| 35:E:55:VAL:O     | 35:E:58:ALA:HB3   | 2.17                     | 0.45              |
| 36:F:49:TYR:O     | 36:F:51:ILE:HG13  | 2.16                     | 0.45              |
| 38:H:8:ASP:C      | 38:H:11:THR:HG22  | 2.41                     | 0.45              |
| 41:K:90:PRO:O     | 41:K:91:GLY:C     | 2.58                     | 0.45              |
| 41:K:120:CYS:SG   | 53:A:677:U:H1'    | 2.57                     | 0.45              |
| 45:O:57:ARG:HG2   | 45:O:57:ARG:HH11  | 1.81                     | 0.45              |
| 49:S:5:LYS:HG3    | 49:S:6:LYS:N      | 2.30                     | 0.45              |
| 53:A:349:A:O2'    | 53:A:350:G:H5'    | 2.16                     | 0.45              |
| 53:A:1352:C:H2'   | 53:A:1353:G:C8    | 2.51                     | 0.45              |
| 53:A:1444:U:H2'   | 53:A:1445:U:C6    | 2.51                     | 0.45              |
| 54:01:381:G:H2'   | 54:01:382:A:H8    | 1.82                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:01:745:G:O2'    | 54:01:748:G:H1'    | 2.17                     | 0.45              |
| 54:01:765:C:H2'    | 54:01:766:U:H6     | 1.79                     | 0.45              |
| 54:01:1348:C:H2'   | 54:01:1349:C:H5'   | 1.97                     | 0.45              |
| 54:01:2263:C:O2'   | 54:01:2264:C:H5'   | 2.16                     | 0.45              |
| 54:01:2516:A:O2'   | 54:01:2517:C:H5'   | 2.16                     | 0.45              |
| 57:V:17:U:H2'      | 57:V:18:G:C8       | 2.52                     | 0.45              |
| 1:04:180:MET:HB2   | 1:04:268:ARG:H     | 1.81                     | 0.45              |
| 4:07:53:ALA:O      | 4:07:64:PRO:HG3    | 2.16                     | 0.45              |
| 4:07:58:ALA:O      | 4:07:59:ILE:C      | 2.60                     | 0.45              |
| 4:07:95:MET:HG3    | 4:07:96:TRP:N      | 2.31                     | 0.45              |
| 5:08:157:LYS:HB2   | 5:08:159:LYS:HG3   | 1.98                     | 0.45              |
| 8:11:15:GLY:C      | 8:11:16:MET:HE2    | 2.42                     | 0.45              |
| 13:16:79:LEU:O     | 13:16:80:PHE:HB2   | 2.16                     | 0.45              |
| 25:28:53:MET:HG3   | 25:28:54:VAL:HG13  | 1.99                     | 0.45              |
| 34:D:169:TRP:CD1   | 34:D:170:LEU:N     | 2.84                     | 0.45              |
| 35:E:45:VAL:CG1    | 35:E:117:ALA:HA    | 2.47                     | 0.45              |
| 35:E:45:VAL:HG11   | 35:E:117:ALA:HA    | 1.99                     | 0.45              |
| 35:E:88:HIS:CE1    | 35:E:89:THR:OG1    | 2.70                     | 0.45              |
| 36:F:103:VAL:HG12  | 36:F:107:ASP:OD2   | 2.17                     | 0.45              |
| 39:I:22:PRO:HA     | 39:I:60:LEU:HB3    | 1.98                     | 0.45              |
| 40:J:30:LYS:HA     | 40:J:34:ALA:CA     | 2.38                     | 0.45              |
| 41:K:34:THR:HB     | 41:K:39:ASN:O      | 2.16                     | 0.45              |
| 43:M:113:LYS:N     | 43:M:114:PRO:CD    | 2.77                     | 0.45              |
| 45:O:86:LEU:HD12   | 45:O:87:ARG:CB     | 2.46                     | 0.45              |
| 46:P:12:LYS:C      | 46:P:14:ARG:H      | 2.24                     | 0.45              |
| 48:R:41:SER:C      | 48:R:43:ILE:N      | 2.74                     | 0.45              |
| 51:U:24:LYS:HG2    | 51:U:25:ALA:H      | 1.80                     | 0.45              |
| 54:01:326:G:H2'    | 54:01:327:G:H8     | 1.81                     | 0.45              |
| 54:01:341:C:H2'    | 54:01:342:A:C8     | 2.52                     | 0.45              |
| 54:01:1932:A:H2'   | 54:01:1933:G:O4'   | 2.16                     | 0.45              |
| 54:01:2832:U:H1'   | 54:01:2834:G:C2    | 2.50                     | 0.45              |
| 4:07:48:LEU:O      | 4:07:51:ASN:HB2    | 2.17                     | 0.45              |
| 6:09:8:LYS:C       | 6:09:13:GLY:HA3    | 2.38                     | 0.45              |
| 8:11:42:ASN:HA     | 8:11:45:THR:HB     | 1.98                     | 0.45              |
| 9:12:34:ARG:HH21   | 16:19:69:ARG:HD2   | 1.80                     | 0.45              |
| 9:12:136:GLN:N     | 9:12:137:PRO:CD    | 2.80                     | 0.45              |
| 14:17:88:LYS:O     | 14:17:115:LEU:HD12 | 2.16                     | 0.45              |
| 14:17:103:VAL:HG23 | 14:17:104:GLN:N    | 2.31                     | 0.45              |
| 22:25:12:SER:OG    | 54:01:2262:U:H5    | 1.99                     | 0.45              |
| 25:28:5:LYS:HB2    | 25:28:57:GLU:HG3   | 1.99                     | 0.45              |
| 27:30:46:GLY:HA3   | 27:30:54:ILE:CG2   | 2.45                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:E:75:LEU:HD12  | 35:E:75:LEU:C      | 2.42                     | 0.45              |
| 46:P:31:ARG:HB2   | 53:A:310:G:H5''    | 1.99                     | 0.45              |
| 50:T:28:ARG:NH1   | 53:A:1437:A:H5''   | 2.32                     | 0.45              |
| 51:U:9:GLU:HB2    | 51:U:10:PRO:HD3    | 1.99                     | 0.45              |
| 54:01:809:G:H2'   | 54:01:810:U:C6     | 2.51                     | 0.45              |
| 54:01:1065:U:H5'  | 54:01:1066:U:OP2   | 2.17                     | 0.45              |
| 54:01:1155:A:O2'  | 54:01:1156:A:H2'   | 2.16                     | 0.45              |
| 54:01:1450:G:O2'  | 54:01:1451:C:H5'   | 2.17                     | 0.45              |
| 54:01:2287:A:N7   | 54:01:2289:G:C8    | 2.84                     | 0.45              |
| 54:01:2515:C:H2'  | 54:01:2516:A:H8    | 1.80                     | 0.45              |
| 1:04:51:ARG:O     | 1:04:53:ILE:HG13   | 2.17                     | 0.45              |
| 2:05:5:VAL:HG11   | 2:05:80:TRP:CZ3    | 2.51                     | 0.45              |
| 2:05:55:LYS:CD    | 2:05:77:ARG:HA     | 2.45                     | 0.45              |
| 3:06:75:SER:OG    | 3:06:76:PRO:HD2    | 2.16                     | 0.45              |
| 4:07:89:THR:O     | 55:02:43:C:H1'     | 2.17                     | 0.45              |
| 8:11:101:SER:HB3  | 8:11:104:GLN:CG    | 2.46                     | 0.45              |
| 9:12:78:THR:HG21  | 54:01:2642:G:P     | 2.56                     | 0.45              |
| 9:12:93:ILE:O     | 9:12:97:PRO:HD3    | 2.17                     | 0.45              |
| 16:19:105:PHE:O   | 16:19:109:VAL:HG23 | 2.17                     | 0.45              |
| 18:21:20:VAL:HG21 | 18:21:43:ALA:HB3   | 1.97                     | 0.45              |
| 33:C:180:ASP:HB3  | 33:C:204:GLY:HA3   | 1.99                     | 0.45              |
| 34:D:79:ALA:HA    | 34:D:85:THR:CG2    | 2.47                     | 0.45              |
| 34:D:169:TRP:HZ3  | 34:D:190:LEU:HB3   | 1.81                     | 0.45              |
| 35:E:108:GLY:C    | 35:E:110:MET:H     | 2.24                     | 0.45              |
| 37:G:17:PHE:O     | 37:G:17:PHE:CD1    | 2.69                     | 0.45              |
| 37:G:58:LEU:H     | 37:G:58:LEU:HD12   | 1.81                     | 0.45              |
| 43:M:66:GLY:HA2   | 43:M:69:ARG:HB2    | 1.98                     | 0.45              |
| 53:A:58:C:O2'     | 53:A:59:A:H5'      | 2.16                     | 0.45              |
| 53:A:476:U:H2'    | 53:A:477:C:C6      | 2.52                     | 0.45              |
| 53:A:604:G:H2'    | 53:A:605:U:O4'     | 2.16                     | 0.45              |
| 53:A:971:G:H4'    | 53:A:972:C:H5'     | 1.98                     | 0.45              |
| 53:A:1405:G:O2'   | 53:A:1406:U:H5'    | 2.17                     | 0.45              |
| 54:01:32:C:H2'    | 54:01:33:C:C6      | 2.52                     | 0.45              |
| 54:01:161:A:H62   | 54:01:165:A:H61    | 1.65                     | 0.45              |
| 54:01:1772:A:H2'  | 54:01:1773:A:H4'   | 1.98                     | 0.45              |
| 54:01:1917:U:O2'  | 54:01:1918:A:H5'   | 2.16                     | 0.45              |
| 54:01:2122:U:H2'  | 54:01:2123:G:O4'   | 2.17                     | 0.45              |
| 55:02:63:C:H2'    | 55:02:64:G:C8      | 2.52                     | 0.45              |
| 1:04:141:HIS:CE1  | 1:04:190:THR:HG22  | 2.52                     | 0.45              |
| 4:07:127:TYR:CE2  | 4:07:129:MET:HE2   | 2.46                     | 0.45              |
| 6:09:117:LEU:HD23 | 6:09:130:VAL:HG13  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:10:18:VAL:HA    | 7:10:86:MET:HE2   | 1.97                     | 0.45              |
| 9:12:40:HIS:CE1   | 9:12:41:LYS:HG3   | 2.51                     | 0.45              |
| 10:13:87:LEU:HA   | 10:13:94:PRO:HA   | 1.98                     | 0.45              |
| 11:14:78:ARG:HB3  | 11:14:113:ALA:CB  | 2.46                     | 0.45              |
| 12:15:125:PRO:HB3 | 54:01:2485:G:O3'  | 2.15                     | 0.45              |
| 13:16:84:GLY:O    | 13:16:88:ALA:N    | 2.50                     | 0.45              |
| 19:22:3:ARG:HH12  | 19:22:7:LEU:HD21  | 1.81                     | 0.45              |
| 19:22:57:VAL:HG22 | 19:22:58:VAL:N    | 2.31                     | 0.45              |
| 21:24:51:GLN:HA   | 21:24:56:PHE:CG   | 2.52                     | 0.45              |
| 21:24:83:LYS:O    | 21:24:85:LYS:N    | 2.46                     | 0.45              |
| 22:25:51:ARG:HH11 | 22:25:51:ARG:HG3  | 1.81                     | 0.45              |
| 36:F:90:MET:SD    | 48:R:22:TYR:CE2   | 3.09                     | 0.45              |
| 41:K:81:LEU:C     | 41:K:81:LEU:HD12  | 2.42                     | 0.45              |
| 53:A:20:U:H2'     | 53:A:21:G:O4'     | 2.17                     | 0.45              |
| 53:A:392:C:H2'    | 53:A:393:A:C8     | 2.50                     | 0.45              |
| 53:A:575:G:O2'    | 53:A:821:G:H5'    | 2.17                     | 0.45              |
| 53:A:1329:A:O2'   | 53:A:1330:U:H5'   | 2.17                     | 0.45              |
| 54:01:1289:C:H2'  | 54:01:1290:C:C6   | 2.51                     | 0.45              |
| 54:01:2520:C:O2'  | 54:01:2521:C:H5'  | 2.17                     | 0.45              |
| 54:01:2679:A:O2'  | 54:01:2680:U:H5'  | 2.17                     | 0.45              |
| 59:Z:144:THR:O    | 59:Z:144:THR:HG23 | 2.16                     | 0.45              |
| 9:12:7:LYS:HG2    | 54:01:538:A:H4'   | 1.99                     | 0.45              |
| 12:15:43:ALA:O    | 12:15:44:ARG:C    | 2.59                     | 0.45              |
| 12:15:50:ARG:HH21 | 12:15:50:ARG:HG2  | 1.82                     | 0.45              |
| 17:20:1:MET:N     | 17:20:43:ASN:HA   | 2.31                     | 0.45              |
| 24:27:23:ARG:O    | 24:27:24:GLU:C    | 2.59                     | 0.45              |
| 24:27:29:ARG:O    | 24:27:32:ALA:HB3  | 2.17                     | 0.45              |
| 26:29:37:CYS:SG   | 26:29:40:CYS:HB3  | 2.57                     | 0.45              |
| 31:34:30:GLU:HA   | 31:34:31:PRO:HD3  | 1.87                     | 0.45              |
| 34:D:27:ILE:O     | 34:D:28:ASP:C     | 2.60                     | 0.45              |
| 38:H:11:THR:HA    | 38:H:14:ARG:HH12  | 1.81                     | 0.45              |
| 41:K:30:ILE:HD13  | 41:K:45:THR:HG22  | 1.98                     | 0.45              |
| 42:L:39:THR:CG2   | 42:L:40:THR:H     | 2.22                     | 0.45              |
| 45:O:44:GLU:HG3   | 45:O:45:HIS:CD2   | 2.51                     | 0.45              |
| 50:T:28:ARG:HH12  | 53:A:1437:A:H5''  | 1.82                     | 0.45              |
| 51:U:58:LYS:HA    | 51:U:61:ARG:CD    | 2.46                     | 0.45              |
| 53:A:321:A:H2'    | 53:A:322:C:C6     | 2.51                     | 0.45              |
| 53:A:680:C:H2'    | 53:A:681:A:C8     | 2.52                     | 0.45              |
| 53:A:902:G:H2'    | 53:A:903:G:C8     | 2.52                     | 0.45              |
| 54:01:20:C:H2'    | 54:01:21:A:C8     | 2.51                     | 0.45              |
| 54:01:112:U:H2'   | 54:01:113:U:H5'   | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:06:12:LEU:CD1   | 3:06:190:ALA:HB1  | 2.47                     | 0.45              |
| 3:06:190:ALA:HA   | 3:06:193:VAL:CG2  | 2.47                     | 0.45              |
| 10:13:110:GLU:HA  | 10:13:113:MET:HB2 | 1.99                     | 0.45              |
| 20:23:73:ASN:C    | 20:23:75:ALA:H    | 2.25                     | 0.45              |
| 26:29:11:GLU:HA   | 26:29:25:ARG:HA   | 1.98                     | 0.45              |
| 32:B:107:ARG:HA   | 32:B:110:ILE:HD12 | 1.98                     | 0.45              |
| 33:C:72:PRO:HA    | 33:C:75:VAL:HB    | 1.99                     | 0.45              |
| 33:C:114:LEU:O    | 33:C:115:VAL:C    | 2.59                     | 0.45              |
| 35:E:9:GLU:HG2    | 35:E:10:LEU:N     | 2.31                     | 0.45              |
| 41:K:51:PHE:O     | 41:K:56:LYS:HB2   | 2.16                     | 0.45              |
| 46:P:20:VAL:CG2   | 46:P:21:VAL:N     | 2.80                     | 0.45              |
| 49:S:62:THR:CG2   | 49:S:63:ASP:H     | 2.19                     | 0.45              |
| 50:T:20:ASN:ND2   | 53:A:323:U:H5'    | 2.31                     | 0.45              |
| 53:A:419:C:H2'    | 53:A:420:U:O4'    | 2.17                     | 0.45              |
| 53:A:1463:U:H2'   | 53:A:1464:U:C6    | 2.52                     | 0.45              |
| 54:01:859:G:C2'   | 54:01:860:U:OP2   | 2.65                     | 0.45              |
| 54:01:1999:C:H2'  | 54:01:2000:C:H6   | 1.82                     | 0.45              |
| 54:01:2025:C:H2'  | 54:01:2026:U:C6   | 2.51                     | 0.45              |
| 1:04:52:HIS:CE1   | 1:04:218:THR:HA   | 2.52                     | 0.45              |
| 2:05:62:LYS:HA    | 2:05:65:ALA:HB3   | 1.98                     | 0.45              |
| 2:05:202:ILE:N    | 2:05:202:ILE:HD12 | 2.31                     | 0.45              |
| 3:06:14:VAL:HG21  | 3:06:19:PHE:CD2   | 2.52                     | 0.45              |
| 5:08:1:SER:C      | 5:08:3:VAL:N      | 2.74                     | 0.45              |
| 6:09:9:VAL:O      | 6:09:10:ALA:C     | 2.60                     | 0.45              |
| 6:09:25:TYR:CE2   | 6:09:30:LEU:HD11  | 2.52                     | 0.45              |
| 7:10:6:GLN:OE1    | 7:10:6:GLN:HA     | 2.17                     | 0.45              |
| 8:11:110:GLN:HA   | 8:11:113:ALA:HB3  | 1.99                     | 0.45              |
| 10:13:49:ARG:HG2  | 10:13:49:ARG:HH11 | 1.82                     | 0.45              |
| 13:16:63:ARG:HH22 | 13:16:80:PHE:HB2  | 1.80                     | 0.45              |
| 13:16:71:ARG:CZ   | 54:01:2708:G:H1'  | 2.47                     | 0.45              |
| 14:17:4:LYS:O     | 14:17:8:ILE:HG13  | 2.17                     | 0.45              |
| 14:17:116:GLN:O   | 14:17:117:PHE:HB3 | 2.17                     | 0.45              |
| 21:24:65:VAL:HG12 | 21:24:68:LYS:O    | 2.16                     | 0.45              |
| 23:26:1:SER:N     | 54:01:1364:G:C8   | 2.84                     | 0.45              |
| 27:30:40:HIS:O    | 27:30:41:HIS:ND1  | 2.50                     | 0.45              |
| 27:30:51:ARG:CG   | 27:30:53:VAL:HG13 | 2.43                     | 0.45              |
| 33:C:61:LYS:O     | 33:C:96:VAL:HB    | 2.16                     | 0.45              |
| 52:03:21:TYR:O    | 52:03:224:VAL:HA  | 2.17                     | 0.45              |
| 52:03:65:LEU:HB2  | 52:03:68:GLY:HA2  | 1.98                     | 0.45              |
| 53:A:1227:A:H2'   | 53:A:1228:C:H5'   | 1.98                     | 0.45              |
| 53:A:1256:A:H1'   | 53:A:1258:G:C4    | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:01:279:A:H2'   | 54:01:280:U:H5'   | 1.98                     | 0.45              |
| 54:01:1441:G:H2'  | 54:01:1442:U:C6   | 2.52                     | 0.45              |
| 54:01:1548:A:H2'  | 54:01:1549:A:H8   | 1.80                     | 0.45              |
| 54:01:2432:A:H1'  | 56:X:75:C:C4'     | 2.47                     | 0.45              |
| 55:02:30:C:H2'    | 55:02:31:C:C5'    | 2.47                     | 0.45              |
| 1:04:69:ASN:HA    | 1:04:188:ARG:NH1  | 2.31                     | 0.44              |
| 1:04:181:ARG:HB3  | 1:04:181:ARG:NH1  | 2.31                     | 0.44              |
| 1:04:245:THR:C    | 1:04:247:TRP:N    | 2.73                     | 0.44              |
| 4:07:140:ILE:N    | 4:07:140:ILE:CD1  | 2.80                     | 0.44              |
| 5:08:169:ARG:HH12 | 54:01:1093:G:C5'  | 2.29                     | 0.44              |
| 8:11:100:ILE:O    | 8:11:140:GLU:HB3  | 2.17                     | 0.44              |
| 11:14:111:ILE:CG2 | 11:14:112:LEU:H   | 2.28                     | 0.44              |
| 14:17:68:LYS:HG3  | 55:02:50:A:OP1    | 2.17                     | 0.44              |
| 14:17:76:LYS:HB2  | 14:17:109:ALA:HB1 | 1.99                     | 0.44              |
| 18:21:59:GLU:CD   | 18:21:66:ILE:HD11 | 2.42                     | 0.44              |
| 20:23:6:ARG:O     | 20:23:24:VAL:HB   | 2.17                     | 0.44              |
| 35:E:105:ILE:HD11 | 35:E:123:LEU:CD2  | 2.47                     | 0.44              |
| 37:G:111:GLY:CA   | 37:G:118:ARG:HH11 | 2.30                     | 0.44              |
| 40:J:35:GLN:HB3   | 40:J:78:GLU:OE2   | 2.16                     | 0.44              |
| 53:A:381:C:H2'    | 53:A:382:A:O4'    | 2.16                     | 0.44              |
| 53:A:1333:A:H2'   | 53:A:1334:G:O4'   | 2.17                     | 0.44              |
| 54:01:123:G:H2'   | 54:01:124:G:O4'   | 2.17                     | 0.44              |
| 54:01:255:A:H2'   | 54:01:256:A:O4'   | 2.17                     | 0.44              |
| 54:01:562:U:H2'   | 54:01:572:A:O4'   | 2.17                     | 0.44              |
| 54:01:753:A:H2'   | 54:01:754:U:C6    | 2.52                     | 0.44              |
| 54:01:1440:U:H2'  | 54:01:1441:G:C8   | 2.51                     | 0.44              |
| 54:01:2241:A:H2'  | 54:01:2242:G:C8   | 2.52                     | 0.44              |
| 54:01:2849:U:H4'  | 54:01:2868:A:C2   | 2.52                     | 0.44              |
| 1:04:90:ILE:O     | 1:04:90:ILE:HG13  | 2.17                     | 0.44              |
| 1:04:205:GLY:O    | 54:01:1791:A:H1'  | 2.17                     | 0.44              |
| 3:06:163:ASN:ND2  | 54:01:320:A:N3    | 2.65                     | 0.44              |
| 3:06:189:THR:HB   | 3:06:192:ALA:HB3  | 1.99                     | 0.44              |
| 7:10:77:VAL:HG22  | 7:10:116:GLU:OE2  | 2.17                     | 0.44              |
| 9:12:95:ARG:HH11  | 9:12:95:ARG:HG3   | 1.82                     | 0.44              |
| 9:12:135:GLN:HB2  | 9:12:137:PRO:HD3  | 1.98                     | 0.44              |
| 12:15:40:ARG:HH12 | 12:15:73:ILE:CD1  | 2.30                     | 0.44              |
| 16:19:7:VAL:HG13  | 16:19:8:ILE:N     | 2.32                     | 0.44              |
| 21:24:26:PHE:CZ   | 21:24:42:LEU:HD11 | 2.52                     | 0.44              |
| 33:C:153:SER:O    | 33:C:196:GLY:N    | 2.51                     | 0.44              |
| 34:D:74:TYR:O     | 34:D:78:ALA:N     | 2.44                     | 0.44              |
| 34:D:120:LYS:HE2  | 34:D:130:ASN:HD21 | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:I:119:LYS:HE2  | 53:A:1349:A:OP1   | 2.16                     | 0.44              |
| 42:L:79:ILE:C     | 42:L:79:ILE:CD1   | 2.90                     | 0.44              |
| 44:N:40:ARG:O     | 44:N:43:ALA:HB3   | 2.17                     | 0.44              |
| 50:T:3:ILE:O      | 50:T:4:LYS:HD2    | 2.17                     | 0.44              |
| 53:A:730:G:H2'    | 53:A:731:G:H5'    | 1.98                     | 0.44              |
| 53:A:1114:C:H2'   | 53:A:1115:U:C6    | 2.53                     | 0.44              |
| 53:A:1202:U:H2'   | 53:A:1203:C:O4'   | 2.17                     | 0.44              |
| 53:A:1271:A:H5'   | 53:A:1314:C:H5''  | 1.98                     | 0.44              |
| 54:01:528:A:C2    | 54:01:2042:A:H2'  | 2.53                     | 0.44              |
| 54:01:779:U:H2'   | 54:01:780:G:C8    | 2.52                     | 0.44              |
| 54:01:1335:C:H2'  | 54:01:1336:A:H8   | 1.82                     | 0.44              |
| 54:01:2246:G:H2'  | 54:01:2247:A:H8   | 1.81                     | 0.44              |
| 54:01:2457:U:O2'  | 54:01:2458:G:H5'  | 2.17                     | 0.44              |
| 56:X:69:C:C2'     | 56:X:70:G:H5'     | 2.47                     | 0.44              |
| 58:Y:74:C:H2'     | 58:Y:75:C:H5'     | 2.00                     | 0.44              |
| 59:Z:150:LYS:CG   | 59:Z:152:LEU:HD23 | 2.47                     | 0.44              |
| 1:04:107:LYS:N    | 1:04:193:GLU:O    | 2.50                     | 0.44              |
| 3:06:187:VAL:HG13 | 3:06:187:VAL:O    | 2.17                     | 0.44              |
| 4:07:121:PHE:CG   | 4:07:162:ASP:HB2  | 2.53                     | 0.44              |
| 4:07:149:ARG:NH1  | 4:07:149:ARG:HB2  | 2.32                     | 0.44              |
| 8:11:89:SER:HB3   | 54:01:1063:G:C2'  | 2.37                     | 0.44              |
| 10:13:41:ILE:C    | 10:13:41:ILE:CD1  | 2.89                     | 0.44              |
| 15:18:63:ILE:HA   | 15:18:68:GLY:HA2  | 2.00                     | 0.44              |
| 16:19:47:ARG:HG2  | 16:19:47:ARG:HH21 | 1.82                     | 0.44              |
| 32:B:138:ARG:NH1  | 32:B:138:ARG:HB2  | 2.32                     | 0.44              |
| 34:D:12:ARG:HD2   | 34:D:36:ALA:O     | 2.17                     | 0.44              |
| 35:E:132:PRO:O    | 35:E:135:VAL:HG22 | 2.16                     | 0.44              |
| 39:I:11:ARG:H     | 39:I:77:ALA:HB2   | 1.83                     | 0.44              |
| 43:M:6:ILE:O      | 43:M:8:ILE:HG13   | 2.17                     | 0.44              |
| 44:N:36:SER:HA    | 44:N:40:ARG:HD2   | 2.00                     | 0.44              |
| 50:T:69:ASN:O     | 50:T:72:ALA:HB3   | 2.17                     | 0.44              |
| 51:U:31:VAL:O     | 51:U:31:VAL:HG22  | 2.17                     | 0.44              |
| 54:01:419:U:H2'   | 54:01:420:C:C6    | 2.53                     | 0.44              |
| 54:01:560:C:H2'   | 54:01:561:G:O4'   | 2.17                     | 0.44              |
| 1:04:245:THR:C    | 1:04:247:TRP:H    | 2.26                     | 0.44              |
| 1:04:270:ARG:CB   | 1:04:270:ARG:NH1  | 2.80                     | 0.44              |
| 4:07:141:ASP:HB2  | 4:07:144:LYS:HD3  | 1.98                     | 0.44              |
| 5:08:71:LEU:HD12  | 5:08:71:LEU:N     | 2.32                     | 0.44              |
| 7:10:60:LEU:HD12  | 7:10:60:LEU:H     | 1.83                     | 0.44              |
| 8:11:53:PRO:O     | 8:11:74:PRO:HD2   | 2.17                     | 0.44              |
| 9:12:101:ILE:N    | 9:12:101:ILE:CD1  | 2.79                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:12:113:PRO:HG3   | 54:01:529:A:OP2    | 2.18                     | 0.44              |
| 12:15:73:ILE:HG12  | 12:15:93:VAL:HG22  | 1.98                     | 0.44              |
| 13:16:108:ALA:HA   | 13:16:109:PRO:HD3  | 1.88                     | 0.44              |
| 23:26:31:ASN:HB2   | 54:01:2230:G:H1'   | 1.99                     | 0.44              |
| 33:C:148:ILE:HG13  | 33:C:201:ILE:HG12  | 1.98                     | 0.44              |
| 35:E:136:VAL:CG1   | 35:E:137:ARG:N     | 2.80                     | 0.44              |
| 39:I:46:VAL:HA     | 39:I:49:GLN:CD     | 2.42                     | 0.44              |
| 40:J:59:LYS:HE2    | 40:J:62:ARG:NH2    | 2.22                     | 0.44              |
| 46:P:37:GLY:HA2    | 46:P:51:ARG:O      | 2.17                     | 0.44              |
| 52:03:44:VAL:HB    | 52:03:173:THR:HG23 | 1.99                     | 0.44              |
| 53:A:56:U:H2'      | 53:A:57:G:H8       | 1.82                     | 0.44              |
| 53:A:948:C:H2'     | 53:A:949:A:C8      | 2.52                     | 0.44              |
| 54:01:214:G:H2'    | 54:01:215:G:C8     | 2.52                     | 0.44              |
| 54:01:490:C:O2'    | 54:01:491:G:P      | 2.76                     | 0.44              |
| 54:01:1797:G:C6    | 54:01:1798:U:C4    | 3.05                     | 0.44              |
| 54:01:2292:U:H2'   | 54:01:2293:G:C8    | 2.51                     | 0.44              |
| 54:01:2411:A:H2'   | 54:01:2412:A:C8    | 2.52                     | 0.44              |
| 54:01:2604:U:H2'   | 54:01:2605:U:C6    | 2.53                     | 0.44              |
| 3:06:121:VAL:HG21  | 3:06:124:PHE:HB2   | 1.99                     | 0.44              |
| 6:09:16:GLY:HA2    | 6:09:47:PHE:HZ     | 1.82                     | 0.44              |
| 12:15:135:VAL:HG21 | 21:24:54:ALA:HB1   | 2.00                     | 0.44              |
| 16:19:32:ARG:O     | 16:19:32:ARG:HG2   | 2.17                     | 0.44              |
| 16:19:57:ARG:HG2   | 16:19:57:ARG:HH11  | 1.83                     | 0.44              |
| 17:20:5:PHE:O      | 17:20:11:GLN:HA    | 2.17                     | 0.44              |
| 17:20:60:LYS:HB2   | 17:20:99:THR:OG1   | 2.17                     | 0.44              |
| 18:21:88:ARG:HG3   | 18:21:88:ARG:HH21  | 1.82                     | 0.44              |
| 25:28:52:PHE:CZ    | 25:28:53:MET:HE2   | 2.51                     | 0.44              |
| 28:31:37:LYS:O     | 28:31:45:HIS:HA    | 2.18                     | 0.44              |
| 33:C:18:ASN:O      | 33:C:55:VAL:HG13   | 2.17                     | 0.44              |
| 33:C:105:VAL:O     | 33:C:105:VAL:HG13  | 2.17                     | 0.44              |
| 33:C:161:ILE:C     | 33:C:161:ILE:CD1   | 2.91                     | 0.44              |
| 35:E:10:LEU:HD12   | 35:E:10:LEU:C      | 2.43                     | 0.44              |
| 36:F:66:ALA:HB1    | 36:F:67:PRO:CD     | 2.41                     | 0.44              |
| 36:F:97:THR:O      | 36:F:98:GLU:CB     | 2.66                     | 0.44              |
| 41:K:111:ASP:CG    | 41:K:113:THR:HG23  | 2.42                     | 0.44              |
| 45:O:71:ARG:HH21   | 53:A:754:C:H5'     | 1.82                     | 0.44              |
| 52:03:220:ALA:HA   | 54:01:2176:A:H5'   | 1.99                     | 0.44              |
| 54:01:528:A:H2     | 54:01:2042:A:H2'   | 1.83                     | 0.44              |
| 54:01:621:A:H2'    | 54:01:622:G:H5'    | 2.00                     | 0.44              |
| 54:01:1219:U:H2'   | 54:01:1220:G:H8    | 1.80                     | 0.44              |
| 54:01:1475:G:O2'   | 54:01:1476:U:H6    | 2.00                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:07:114:ARG:HG3   | 4:07:177:ARG:HD3  | 1.98                     | 0.44              |
| 5:08:67:ALA:HA     | 5:08:70:LEU:HD12  | 2.00                     | 0.44              |
| 10:13:20:MET:O     | 10:13:41:ILE:HB   | 2.18                     | 0.44              |
| 10:13:108:ARG:HH11 | 10:13:113:MET:HE1 | 1.82                     | 0.44              |
| 18:21:42:LYS:NZ    | 18:21:46:LEU:HD11 | 2.32                     | 0.44              |
| 21:24:5:ASN:HA     | 21:24:64:VAL:HB   | 1.99                     | 0.44              |
| 35:E:164:LEU:HD12  | 35:E:164:LEU:C    | 2.41                     | 0.44              |
| 40:J:10:LEU:CD1    | 40:J:18:ILE:HD11  | 2.48                     | 0.44              |
| 43:M:109:LYS:HD2   | 53:A:1227:A:OP2   | 2.17                     | 0.44              |
| 44:N:9:GLU:O       | 44:N:13:VAL:HG23  | 2.18                     | 0.44              |
| 45:O:70:LYS:HD3    | 45:O:77:TYR:CE2   | 2.53                     | 0.44              |
| 50:T:43:LYS:HD3    | 50:T:86:ALA:HB1   | 1.98                     | 0.44              |
| 53:A:146:G:H2'     | 53:A:147:G:C8     | 2.53                     | 0.44              |
| 54:01:415:A:H2'    | 54:01:416:U:C6    | 2.53                     | 0.44              |
| 54:01:996:A:H2'    | 54:01:997:G:C8    | 2.51                     | 0.44              |
| 54:01:1935:G:H2'   | 54:01:1962:C:H42  | 1.83                     | 0.44              |
| 54:01:2467:C:H2'   | 54:01:2468:A:O4'  | 2.18                     | 0.44              |
| 54:01:2661:G:H2'   | 54:01:2662:A:O4'  | 2.18                     | 0.44              |
| 55:02:60:C:H2'     | 55:02:61:G:H8     | 1.82                     | 0.44              |
| 1:04:164:VAL:HG21  | 1:04:180:MET:HE1  | 1.99                     | 0.44              |
| 7:10:99:PHE:O      | 7:10:103:ASN:N    | 2.50                     | 0.44              |
| 8:11:23:VAL:HG11   | 8:11:27:LEU:HD23  | 2.00                     | 0.44              |
| 8:11:72:THR:HG23   | 8:11:73:PRO:HD2   | 2.00                     | 0.44              |
| 12:15:55:ARG:HG3   | 12:15:55:ARG:HH21 | 1.83                     | 0.44              |
| 22:25:19:VAL:HG22  | 22:25:34:VAL:CG2  | 2.47                     | 0.44              |
| 22:25:19:VAL:HG13  | 22:25:34:VAL:HG22 | 2.00                     | 0.44              |
| 35:E:84:VAL:HG22   | 35:E:85:LYS:N     | 2.32                     | 0.44              |
| 43:M:65:GLU:HG3    | 43:M:66:GLY:N     | 2.29                     | 0.44              |
| 44:N:5:MET:HE3     | 44:N:62:ARG:HH21  | 1.82                     | 0.44              |
| 47:Q:24:ILE:N      | 47:Q:41:THR:O     | 2.51                     | 0.44              |
| 49:S:23:GLU:HG3    | 49:S:24:SER:N     | 2.33                     | 0.44              |
| 53:A:319:G:H2'     | 53:A:320:A:H8     | 1.82                     | 0.44              |
| 53:A:620:C:H2'     | 53:A:621:A:O4'    | 2.18                     | 0.44              |
| 53:A:622:A:H2'     | 53:A:623:C:H5'    | 2.00                     | 0.44              |
| 54:01:480:A:H3'    | 54:01:481:G:H5''  | 2.00                     | 0.44              |
| 54:01:727:A:C2'    | 54:01:728:G:H5'   | 2.48                     | 0.44              |
| 54:01:876:C:H2'    | 54:01:877:A:O4'   | 2.17                     | 0.44              |
| 54:01:1394:U:H4'   | 54:01:1603:A:H4'  | 2.00                     | 0.44              |
| 58:Y:25:C:H2'      | 58:Y:26:A:C8      | 2.52                     | 0.44              |
| 58:Y:63:G:O2'      | 58:Y:64:A:OP1     | 2.35                     | 0.44              |
| 1:04:129:LEU:HD12  | 1:04:130:PRO:O    | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:05:109:VAL:HG11 | 2:05:193:VAL:HB   | 2.00                     | 0.44              |
| 7:10:3:LEU:H      | 7:10:6:GLN:HB2    | 1.83                     | 0.44              |
| 7:10:55:VAL:HG13  | 54:01:1084:A:OP1  | 2.18                     | 0.44              |
| 9:12:58:ASN:HD22  | 9:12:58:ASN:HA    | 1.62                     | 0.44              |
| 9:12:84:ILE:HD12  | 9:12:85:LYS:N     | 2.33                     | 0.44              |
| 10:13:25:LEU:CD2  | 54:01:2562:U:H4'  | 2.48                     | 0.44              |
| 10:13:62:VAL:HG12 | 10:13:63:VAL:N    | 2.33                     | 0.44              |
| 18:21:3:THR:HG21  | 18:21:58:ALA:CA   | 2.47                     | 0.44              |
| 20:23:82:VAL:CG1  | 20:23:83:GLY:H    | 2.20                     | 0.44              |
| 23:26:53:LYS:O    | 23:26:57:VAL:HG23 | 2.18                     | 0.44              |
| 37:G:55:LYS:HB2   | 37:G:60:ALA:CB    | 2.47                     | 0.44              |
| 38:H:11:THR:HG23  | 38:H:12:ARG:N     | 2.32                     | 0.44              |
| 38:H:90:GLU:HG2   | 38:H:90:GLU:O     | 2.18                     | 0.44              |
| 39:I:25:GLY:O     | 39:I:27:ILE:CD1   | 2.65                     | 0.44              |
| 42:L:73:LEU:HD12  | 42:L:73:LEU:H     | 1.82                     | 0.44              |
| 44:N:53:ASP:O     | 44:N:54:SER:HB3   | 2.16                     | 0.44              |
| 45:O:86:LEU:O     | 45:O:87:ARG:HB3   | 2.18                     | 0.44              |
| 46:P:69:ASP:O     | 46:P:70:ARG:C     | 2.61                     | 0.44              |
| 53:A:342:C:O2'    | 53:A:343:U:H5'    | 2.18                     | 0.44              |
| 53:A:824:G:H2'    | 53:A:825:A:C8     | 2.50                     | 0.44              |
| 53:A:1001:C:H2'   | 53:A:1002:G:H8    | 1.83                     | 0.44              |
| 53:A:1137:C:H5'   | 53:A:1138:G:H5'   | 2.00                     | 0.44              |
| 53:A:1497:G:O2'   | 53:A:1498:U:H5'   | 2.18                     | 0.44              |
| 54:01:181:A:H2'   | 54:01:182:A:H8    | 1.82                     | 0.44              |
| 54:01:254:G:O2'   | 54:01:255:A:H5''  | 2.18                     | 0.44              |
| 54:01:443:A:H5''  | 54:01:444:C:C5'   | 2.47                     | 0.44              |
| 54:01:941:A:H2'   | 54:01:942:G:O4'   | 2.18                     | 0.44              |
| 59:Z:101:ALA:HB1  | 59:Z:106:GLU:CG   | 2.47                     | 0.44              |
| 1:04:260:LYS:O    | 1:04:261:ARG:C    | 2.60                     | 0.44              |
| 2:05:40:LEU:N     | 2:05:40:LEU:HD12  | 2.33                     | 0.44              |
| 2:05:62:LYS:O     | 2:05:63:PRO:C     | 2.61                     | 0.44              |
| 2:05:101:PHE:HA   | 2:05:104:VAL:HG22 | 2.00                     | 0.44              |
| 8:11:128:ILE:H    | 8:11:128:ILE:CD1  | 2.29                     | 0.44              |
| 9:12:42:ALA:O     | 16:19:63:ARG:HD2  | 2.18                     | 0.44              |
| 14:17:101:GLY:O   | 14:17:102:ARG:C   | 2.60                     | 0.44              |
| 18:21:42:LYS:HB2  | 54:01:2010:G:C5'  | 2.47                     | 0.44              |
| 25:28:13:ILE:C    | 25:28:15:ARG:H    | 2.26                     | 0.44              |
| 33:C:48:LYS:HD2   | 33:C:48:LYS:N     | 2.33                     | 0.44              |
| 34:D:18:LEU:O     | 34:D:19:PHE:HB2   | 2.17                     | 0.44              |
| 35:E:47:PHE:CZ    | 35:E:137:ARG:HG2  | 2.53                     | 0.44              |
| 42:L:31:GLY:HA3   | 42:L:54:VAL:HG12  | 1.96                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:03:27:ILE:HD12 | 52:03:182:ALA:HB1  | 1.99                     | 0.44              |
| 53:A:114:U:O2'    | 53:A:115:G:H5'     | 2.18                     | 0.44              |
| 54:01:729:G:H2'   | 54:01:729:G:N3     | 2.33                     | 0.44              |
| 54:01:2176:A:H2'  | 54:01:2177:C:C6    | 2.53                     | 0.44              |
| 59:Z:150:LYS:HB3  | 59:Z:150:LYS:HZ3   | 1.83                     | 0.44              |
| 5:08:41:GLU:HB2   | 5:08:54:ARG:HB2    | 1.99                     | 0.43              |
| 7:10:37:LYS:HB2   | 7:10:41:LEU:HD12   | 1.99                     | 0.43              |
| 8:11:27:LEU:HD12  | 8:11:28:GLY:H      | 1.76                     | 0.43              |
| 9:12:80:HIS:O     | 9:12:81:ILE:C      | 2.61                     | 0.43              |
| 12:15:42:THR:HA   | 12:15:93:VAL:HG12  | 2.00                     | 0.43              |
| 13:16:2:ARG:HA    | 13:16:5:LYS:CE     | 2.48                     | 0.43              |
| 13:16:90:ARG:CZ   | 13:16:116:VAL:HG11 | 2.48                     | 0.43              |
| 17:20:49:ILE:HD12 | 17:20:52:PRO:CA    | 2.48                     | 0.43              |
| 17:20:88:GLY:O    | 17:20:89:HIS:HB2   | 2.17                     | 0.43              |
| 18:21:7:HIS:CD2   | 18:21:10:ALA:HB2   | 2.53                     | 0.43              |
| 22:25:64:LYS:HG3  | 22:25:65:PHE:N     | 2.32                     | 0.43              |
| 26:29:56:ARG:HH22 | 49:S:68:HIS:CE1    | 2.27                     | 0.43              |
| 32:B:13:VAL:HG13  | 32:B:212:TYR:OH    | 2.18                     | 0.43              |
| 33:C:9:ILE:CD1    | 44:N:97:LYS:HD3    | 2.43                     | 0.43              |
| 33:C:24:ASN:O     | 33:C:28:PHE:HB2    | 2.18                     | 0.43              |
| 33:C:129:PHE:O    | 33:C:133:MET:N     | 2.44                     | 0.43              |
| 38:H:1:SER:O      | 38:H:2:MET:C       | 2.61                     | 0.43              |
| 46:P:20:VAL:HG23  | 46:P:34:GLU:C      | 2.44                     | 0.43              |
| 51:U:66:ARG:HA    | 51:U:66:ARG:HD3    | 1.82                     | 0.43              |
| 52:03:43:ASP:HA   | 52:03:174:THR:HG22 | 2.00                     | 0.43              |
| 53:A:45:G:H5''    | 53:A:307:C:O2'     | 2.18                     | 0.43              |
| 53:A:599:C:H2'    | 53:A:600:A:H8      | 1.83                     | 0.43              |
| 53:A:740:U:O2'    | 53:A:741:G:H5'     | 2.18                     | 0.43              |
| 53:A:742:G:O2'    | 53:A:743:A:H5'     | 2.18                     | 0.43              |
| 53:A:757:U:H2'    | 53:A:758:C:O4'     | 2.17                     | 0.43              |
| 54:01:52:A:O2'    | 54:01:53:A:H5'     | 2.18                     | 0.43              |
| 54:01:288:U:H2'   | 54:01:289:G:H8     | 1.83                     | 0.43              |
| 54:01:974:G:H2'   | 54:01:974:G:N3     | 2.32                     | 0.43              |
| 2:05:110:THR:HG23 | 2:05:171:THR:OG1   | 2.18                     | 0.43              |
| 3:06:109:LEU:HD12 | 3:06:109:LEU:N     | 2.32                     | 0.43              |
| 5:08:2:ARG:HA     | 5:08:5:LYS:HZ3     | 1.82                     | 0.43              |
| 7:10:97:LYS:O     | 7:10:100:ALA:HB3   | 2.18                     | 0.43              |
| 8:11:19:PRO:C     | 8:11:22:PRO:HD2    | 2.43                     | 0.43              |
| 13:16:45:ARG:C    | 13:16:47:VAL:H     | 2.26                     | 0.43              |
| 15:18:13:LYS:HE3  | 15:18:76:HIS:HA    | 1.98                     | 0.43              |
| 15:18:92:ARG:HD3  | 54:01:1753:G:OP1   | 2.17                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:19:60:TRP:CZ2  | 16:19:92:LYS:HG3  | 2.53                     | 0.43              |
| 19:22:48:GLN:NE2  | 19:22:55:VAL:H    | 2.16                     | 0.43              |
| 20:23:86:PHE:CE1  | 20:23:91:LYS:HE2  | 2.53                     | 0.43              |
| 36:F:51:ILE:O     | 36:F:52:ASN:C     | 2.62                     | 0.43              |
| 39:I:70:GLY:O     | 39:I:74:GLN:HG3   | 2.18                     | 0.43              |
| 43:M:37:GLY:O     | 43:M:38:ILE:HD13  | 2.18                     | 0.43              |
| 47:Q:21:VAL:HG13  | 47:Q:21:VAL:O     | 2.17                     | 0.43              |
| 47:Q:58:VAL:HG22  | 47:Q:59:GLU:N     | 2.33                     | 0.43              |
| 48:R:12:PHE:CE2   | 48:R:20:ILE:HD11  | 2.53                     | 0.43              |
| 51:U:65:ARG:HB2   | 51:U:67:THR:CG2   | 2.46                     | 0.43              |
| 53:A:651:C:H2'    | 53:A:652:U:C6     | 2.53                     | 0.43              |
| 53:A:663:A:H5'    | 53:A:836:G:OP1    | 2.17                     | 0.43              |
| 53:A:1138:G:H3'   | 53:A:1138:G:N3    | 2.33                     | 0.43              |
| 53:A:1254:A:H2'   | 53:A:1255:G:H8    | 1.83                     | 0.43              |
| 54:01:953:G:H2'   | 54:01:954:G:H8    | 1.83                     | 0.43              |
| 54:01:1330:C:O2'  | 54:01:1331:G:H5'  | 2.17                     | 0.43              |
| 54:01:2282:G:H4'  | 54:01:2389:G:O2'  | 2.18                     | 0.43              |
| 54:01:2623:G:H2'  | 54:01:2624:G:C8   | 2.51                     | 0.43              |
| 54:01:2756:U:H4'  | 54:01:2757:A:OP1  | 2.17                     | 0.43              |
| 54:01:2833:U:O2'  | 54:01:2834:G:H5'  | 2.18                     | 0.43              |
| 1:04:44:ASN:ND2   | 54:01:1812:U:H1'  | 2.32                     | 0.43              |
| 1:04:62:ARG:O     | 1:04:64:VAL:HG23  | 2.18                     | 0.43              |
| 1:04:109:LEU:HD12 | 1:04:113:ASP:OD2  | 2.18                     | 0.43              |
| 1:04:216:ARG:NH2  | 54:01:690:G:O3'   | 2.51                     | 0.43              |
| 3:06:7:ASP:O      | 3:06:9:GLN:HG3    | 2.17                     | 0.43              |
| 4:07:10:GLU:O     | 4:07:13:LYS:HB3   | 2.19                     | 0.43              |
| 4:07:56:LEU:HD23  | 4:07:59:ILE:HD12  | 2.00                     | 0.43              |
| 5:08:37:ASN:HD22  | 5:08:39:ALA:HB3   | 1.83                     | 0.43              |
| 5:08:137:LYS:HA   | 5:08:140:ILE:HD11 | 2.00                     | 0.43              |
| 6:09:114:GLU:HB3  | 6:09:133:GLN:O    | 2.18                     | 0.43              |
| 6:09:132:PHE:HE2  | 6:09:142:VAL:HB   | 1.84                     | 0.43              |
| 7:10:96:PHE:CE2   | 7:10:126:LEU:HB2  | 2.53                     | 0.43              |
| 9:12:54:ILE:HG22  | 9:12:55:ILE:N     | 2.34                     | 0.43              |
| 12:15:45:GLN:HE21 | 54:01:2485:G:C5'  | 2.22                     | 0.43              |
| 15:18:20:ARG:HB3  | 15:18:21:PRO:HD2  | 2.01                     | 0.43              |
| 18:21:93:ALA:HB2  | 54:01:1614:A:N1   | 2.33                     | 0.43              |
| 19:22:77:ARG:HH11 | 19:22:77:ARG:HG3  | 1.83                     | 0.43              |
| 29:32:3:ARG:HG2   | 54:01:1613:G:H4'  | 2.00                     | 0.43              |
| 33:C:131:ARG:NE   | 33:C:135:ARG:HH21 | 2.05                     | 0.43              |
| 34:D:99:ASN:OD1   | 34:D:110:ARG:NH1  | 2.49                     | 0.43              |
| 35:E:56:PRO:HG2   | 35:E:57:ALA:H     | 1.82                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:E:100:GLU:C     | 35:E:102:THR:H    | 2.26                     | 0.43              |
| 37:G:58:LEU:HD12   | 37:G:58:LEU:N     | 2.33                     | 0.43              |
| 37:G:90:VAL:HG23   | 37:G:94:ARG:HD3   | 2.00                     | 0.43              |
| 39:I:91:GLU:O      | 39:I:92:SER:C     | 2.62                     | 0.43              |
| 40:J:42:LEU:HD11   | 40:J:73:LEU:HG    | 2.00                     | 0.43              |
| 41:K:35:ASP:OD1    | 41:K:39:ASN:HB2   | 2.18                     | 0.43              |
| 45:O:48:ASP:O      | 45:O:51:SER:N     | 2.51                     | 0.43              |
| 46:P:23:ASP:OD2    | 46:P:25:ARG:HB2   | 2.18                     | 0.43              |
| 48:R:62:ARG:HB3    | 48:R:69:TYR:CE1   | 2.53                     | 0.43              |
| 52:O3:209:ILE:HG13 | 52:O3:209:ILE:O   | 2.18                     | 0.43              |
| 53:A:36:C:H2'      | 53:A:37:U:O4'     | 2.18                     | 0.43              |
| 53:A:1258:G:H2'    | 53:A:1259:C:C6    | 2.54                     | 0.43              |
| 54:O1:12:U:H2'     | 54:O1:13:A:H5'    | 2.00                     | 0.43              |
| 54:O1:801:G:H3'    | 54:O1:802:A:H5'   | 2.00                     | 0.43              |
| 54:O1:1335:C:H2'   | 54:O1:1336:A:C8   | 2.53                     | 0.43              |
| 54:O1:1893:C:H2'   | 54:O1:1894:C:H5'  | 2.00                     | 0.43              |
| 54:O1:2581:G:H2'   | 54:O1:2581:G:N3   | 2.33                     | 0.43              |
| 56:W:62:C:H2'      | 56:W:63:G:H8      | 1.83                     | 0.43              |
| 2:O5:144:GLY:O     | 2:O5:145:SER:C    | 2.61                     | 0.43              |
| 2:O5:152:PRO:HD3   | 54:O1:2571:U:O2'  | 2.19                     | 0.43              |
| 3:O6:23:PHE:HB2    | 3:O6:114:ARG:NH2  | 2.33                     | 0.43              |
| 3:O6:84:THR:HG21   | 54:O1:586:A:C5'   | 2.48                     | 0.43              |
| 4:O7:91:ARG:CA     | 4:O7:95:MET:HB3   | 2.47                     | 0.43              |
| 6:O9:89:LYS:O      | 6:O9:90:LEU:C     | 2.61                     | 0.43              |
| 8:11:85:ILE:HD13   | 8:11:87:SER:OG    | 2.18                     | 0.43              |
| 8:11:118:GLY:HA3   | 8:11:124:MET:CG   | 2.47                     | 0.43              |
| 12:15:135:VAL:HG21 | 21:24:54:ALA:CB   | 2.48                     | 0.43              |
| 15:18:4:ILE:O      | 15:18:5:LYS:C     | 2.60                     | 0.43              |
| 15:18:28:LYS:HB2   | 15:18:82:SER:OG   | 2.18                     | 0.43              |
| 15:18:52:ARG:HD3   | 54:O1:2845:U:H5'' | 2.01                     | 0.43              |
| 20:23:8:ASP:OD2    | 20:23:71:ILE:HG22 | 2.17                     | 0.43              |
| 27:30:12:ARG:HH11  | 27:30:12:ARG:HG2  | 1.83                     | 0.43              |
| 33:C:133:MET:CE    | 33:C:167:TYR:HB2  | 2.43                     | 0.43              |
| 34:D:168:THR:O     | 34:D:170:LEU:N    | 2.51                     | 0.43              |
| 39:I:64:ILE:HD13   | 39:I:78:ILE:CG2   | 2.49                     | 0.43              |
| 41:K:28:ASN:CG     | 41:K:29:THR:H     | 2.26                     | 0.43              |
| 46:P:33:ILE:H      | 46:P:33:ILE:CD1   | 2.32                     | 0.43              |
| 48:R:13:THR:O      | 48:R:14:ALA:C     | 2.61                     | 0.43              |
| 53:A:45:G:H2'      | 53:A:46:G:C8      | 2.53                     | 0.43              |
| 53:A:212:G:H2'     | 53:A:213:G:C8     | 2.53                     | 0.43              |
| 53:A:1305:G:H1'    | 53:A:1332:A:N6    | 2.34                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:A:1490:U:O2'   | 53:A:1491:G:H5'   | 2.18                     | 0.43              |
| 54:01:20:C:H2'    | 54:01:21:A:H8     | 1.83                     | 0.43              |
| 54:01:542:C:C2'   | 54:01:543:G:H5''  | 2.48                     | 0.43              |
| 54:01:774:G:H2'   | 54:01:775:G:H5''  | 1.98                     | 0.43              |
| 54:01:864:G:O2'   | 54:01:865:C:H5'   | 2.18                     | 0.43              |
| 54:01:1063:G:H3'  | 54:01:1063:G:H8   | 1.83                     | 0.43              |
| 54:01:1652:A:C2'  | 54:01:1653:G:H5'  | 2.48                     | 0.43              |
| 54:01:2606:C:H2'  | 54:01:2607:G:C8   | 2.53                     | 0.43              |
| 54:01:2834:G:O2'  | 54:01:2835:A:H5'  | 2.19                     | 0.43              |
| 59:Z:50:ALA:O     | 59:Z:54:LYS:HG3   | 2.18                     | 0.43              |
| 1:04:154:ALA:HA   | 1:04:159:THR:CG2  | 2.45                     | 0.43              |
| 2:05:109:VAL:O    | 2:05:171:THR:HG23 | 2.19                     | 0.43              |
| 3:06:190:ALA:O    | 3:06:193:VAL:HB   | 2.19                     | 0.43              |
| 4:07:105:ILE:HG13 | 4:07:106:ALA:N    | 2.33                     | 0.43              |
| 5:08:163:TYR:HB2  | 5:08:166:GLU:CB   | 2.49                     | 0.43              |
| 6:09:62:LEU:HA    | 6:09:65:ALA:HB3   | 2.01                     | 0.43              |
| 7:10:59:LEU:HB3   | 7:10:62:ARG:HB2   | 1.99                     | 0.43              |
| 9:12:37:ARG:HG3   | 9:12:37:ARG:NH2   | 2.33                     | 0.43              |
| 10:13:4:GLU:HA    | 10:13:21:CYS:O    | 2.19                     | 0.43              |
| 10:13:49:ARG:O    | 10:13:50:GLY:C    | 2.61                     | 0.43              |
| 11:14:65:GLY:HA2  | 54:01:2415:G:O3'  | 2.18                     | 0.43              |
| 12:15:17:ASN:HB2  | 12:15:95:LEU:HD22 | 2.01                     | 0.43              |
| 13:16:97:ILE:O    | 13:16:98:LEU:HD23 | 2.18                     | 0.43              |
| 17:20:6:GLN:O     | 17:20:37:GLU:HG3  | 2.18                     | 0.43              |
| 18:21:25:ARG:HH11 | 18:21:25:ARG:HG3  | 1.84                     | 0.43              |
| 20:23:31:GLY:C    | 20:23:66:VAL:HG23 | 2.44                     | 0.43              |
| 29:32:25:LYS:O    | 29:32:26:ASN:C    | 2.61                     | 0.43              |
| 33:C:61:LYS:O     | 33:C:97:PRO:HD2   | 2.18                     | 0.43              |
| 36:F:17:GLN:O     | 36:F:21:MET:HG3   | 2.17                     | 0.43              |
| 36:F:32:ALA:O     | 36:F:33:GLU:HB2   | 2.18                     | 0.43              |
| 38:H:24:VAL:O     | 38:H:59:GLU:HA    | 2.19                     | 0.43              |
| 42:L:26:CYS:SG    | 42:L:29:LYS:HD3   | 2.57                     | 0.43              |
| 48:R:48:ALA:O     | 48:R:49:LYS:C     | 2.62                     | 0.43              |
| 50:T:80:ALA:O     | 50:T:84:LYS:HB2   | 2.19                     | 0.43              |
| 52:03:38:PHE:CE2  | 54:01:2127:G:H4'  | 2.53                     | 0.43              |
| 53:A:21:G:H2'     | 53:A:22:G:C8      | 2.53                     | 0.43              |
| 53:A:556:C:O2'    | 53:A:557:G:H5'    | 2.19                     | 0.43              |
| 53:A:1081:A:O2'   | 53:A:1082:A:H5'   | 2.19                     | 0.43              |
| 54:01:28:A:H1'    | 54:01:513:A:C2    | 2.53                     | 0.43              |
| 54:01:341:C:H2'   | 54:01:342:A:H8    | 1.83                     | 0.43              |
| 54:01:696:G:O2'   | 54:01:697:G:H5'   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 54:01:813:U:H2'   | 54:01:814:C:H6   | 1.83                     | 0.43              |
| 54:01:912:C:O2'   | 54:01:913:U:H5'  | 2.19                     | 0.43              |
| 54:01:1201:U:H2'  | 54:01:1202:G:H8  | 1.83                     | 0.43              |
| 54:01:1316:U:H2'  | 54:01:1317:G:H8  | 1.83                     | 0.43              |
| 54:01:1516:G:O2'  | 54:01:1517:G:H5' | 2.19                     | 0.43              |
| 54:01:1794:A:H2'  | 54:01:1795:C:H6  | 1.83                     | 0.43              |
| 54:01:1917:U:C2'  | 54:01:1918:A:H5' | 2.49                     | 0.43              |
| 54:01:2846:G:H2'  | 54:01:2847:U:O4' | 2.18                     | 0.43              |
| 4:07:148:VAL:HG12 | 4:07:148:VAL:O   | 2.19                     | 0.43              |
| 5:08:173:ALA:O    | 5:08:174:LYS:C   | 2.62                     | 0.43              |
| 9:12:95:ARG:HG2   | 9:12:96:ARG:HG3  | 2.01                     | 0.43              |
| 14:17:56:LYS:O    | 14:17:60:GLU:HG3 | 2.19                     | 0.43              |
| 15:18:23:ASP:OD1  | 15:18:88:ARG:HA  | 2.18                     | 0.43              |
| 18:21:83:LYS:O    | 18:21:84:ARG:NH2 | 2.50                     | 0.43              |
| 32:B:137:THR:O    | 32:B:140:LEU:HB3 | 2.19                     | 0.43              |
| 34:D:193:ASP:OD1  | 34:D:194:ILE:N   | 2.52                     | 0.43              |
| 38:H:29:SER:O     | 38:H:32:LYS:HB2  | 2.19                     | 0.43              |
| 39:I:119:LYS:C    | 39:I:121:ARG:H   | 2.25                     | 0.43              |
| 51:U:18:PHE:HA    | 51:U:21:SER:HB3  | 2.00                     | 0.43              |
| 53:A:1256:A:H4'   | 53:A:1258:G:O4'  | 2.19                     | 0.43              |
| 54:01:1092:C:H2'  | 54:01:1093:G:O4' | 2.19                     | 0.43              |
| 54:01:1344:U:O2   | 54:01:1385:A:H5' | 2.19                     | 0.43              |
| 54:01:1441:G:H4'  | 54:01:1628:G:H5' | 2.01                     | 0.43              |
| 54:01:1736:U:H2'  | 54:01:1737:G:O4' | 2.19                     | 0.43              |
| 54:01:2144:G:H1'  | 54:01:2147:A:H61 | 1.84                     | 0.43              |
| 54:01:2590:A:O2'  | 54:01:2591:C:H5' | 2.19                     | 0.43              |
| 54:01:2628:C:H3'  | 54:01:2629:U:H5' | 2.00                     | 0.43              |
| 58:Y:59:U:C2'     | 58:Y:60:U:H5'    | 2.49                     | 0.43              |
| 2:05:11:MET:HG2   | 2:05:25:THR:HA   | 2.01                     | 0.43              |
| 2:05:85:ALA:O     | 2:05:86:GLU:HB3  | 2.17                     | 0.43              |
| 11:14:57:LEU:HD22 | 30:33:53:ASP:HB3 | 2.00                     | 0.43              |
| 13:16:103:ARG:HD2 | 13:16:106:ASP:CG | 2.43                     | 0.43              |
| 15:18:52:ARG:HG3  | 15:18:52:ARG:NH1 | 2.33                     | 0.43              |
| 20:23:4:ILE:H     | 20:23:4:ILE:CD1  | 2.29                     | 0.43              |
| 33:C:28:PHE:CD2   | 44:N:75:LYS:HE2  | 2.53                     | 0.43              |
| 33:C:118:SER:O    | 33:C:122:GLN:HG3 | 2.19                     | 0.43              |
| 36:F:18:VAL:O     | 36:F:21:MET:N    | 2.52                     | 0.43              |
| 39:I:16:ALA:HB2   | 39:I:66:VAL:CG2  | 2.48                     | 0.43              |
| 40:J:15:HIS:CG    | 40:J:16:ARG:N    | 2.86                     | 0.43              |
| 40:J:59:LYS:HD3   | 53:A:973:G:OP1   | 2.18                     | 0.43              |
| 42:L:2:THR:HG21   | 42:L:5:GLN:HG3   | 1.98                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:M:13:HIS:O     | 43:M:14:ALA:C     | 2.61                     | 0.43              |
| 43:M:71:GLU:O     | 43:M:74:MET:HB3   | 2.18                     | 0.43              |
| 49:S:35:ARG:HH21  | 49:S:74:ALA:HB3   | 1.84                     | 0.43              |
| 52:03:30:LEU:HD12 | 52:03:31:LYS:N    | 2.32                     | 0.43              |
| 53:A:976:G:N2     | 53:A:1362:A:H2'   | 2.34                     | 0.43              |
| 53:A:1500:A:H5''  | 53:A:1508:A:H5''  | 2.00                     | 0.43              |
| 54:01:182:A:O2'   | 54:01:183:C:H5'   | 2.17                     | 0.43              |
| 54:01:239:C:H2'   | 54:01:240:C:O4'   | 2.18                     | 0.43              |
| 54:01:395:U:H2'   | 54:01:396:G:C8    | 2.54                     | 0.43              |
| 54:01:480:A:H2'   | 54:01:481:G:OP1   | 2.19                     | 0.43              |
| 54:01:1279:G:H2'  | 54:01:1280:G:C8   | 2.54                     | 0.43              |
| 54:01:1561:C:H2'  | 54:01:1562:U:C6   | 2.54                     | 0.43              |
| 54:01:1678:A:H2'  | 54:01:1679:A:O4'  | 2.18                     | 0.43              |
| 54:01:2713:U:H3'  | 54:01:2714:G:H5'' | 2.00                     | 0.43              |
| 55:02:3:C:H3'     | 55:02:4:C:H5''    | 2.01                     | 0.43              |
| 59:Z:122:VAL:HB   | 59:Z:129:ALA:HB3  | 1.99                     | 0.43              |
| 1:04:76:VAL:HG12  | 1:04:77:VAL:N     | 2.34                     | 0.43              |
| 1:04:93:VAL:HG21  | 1:04:103:ILE:CD1  | 2.49                     | 0.43              |
| 1:04:267:VAL:HG12 | 1:04:268:ARG:NH1  | 2.33                     | 0.43              |
| 3:06:149:ILE:CG2  | 3:06:188:MET:HA   | 2.45                     | 0.43              |
| 5:08:85:LYS:C     | 5:08:86:LEU:HD12  | 2.43                     | 0.43              |
| 7:10:22:ALA:HB1   | 7:10:91:ALA:HA    | 2.00                     | 0.43              |
| 7:10:117:LEU:C    | 7:10:119:PRO:CD   | 2.92                     | 0.43              |
| 13:16:40:LYS:HG3  | 54:01:1651:G:OP1  | 2.19                     | 0.43              |
| 13:16:63:ARG:O    | 13:16:66:ALA:HB3  | 2.19                     | 0.43              |
| 15:18:57:ALA:HB1  | 15:18:73:PHE:O    | 2.19                     | 0.43              |
| 16:19:30:VAL:HG13 | 54:01:581:C:OP1   | 2.19                     | 0.43              |
| 20:23:96:LYS:O    | 20:23:98:ASN:N    | 2.52                     | 0.43              |
| 32:B:119:GLN:HB3  | 32:B:124:THR:HB   | 2.01                     | 0.43              |
| 33:C:206:ILE:OXT  | 33:C:206:ILE:HG12 | 2.19                     | 0.43              |
| 34:D:100:VAL:O    | 34:D:104:MET:HG2  | 2.19                     | 0.43              |
| 38:H:63:LYS:O     | 38:H:70:VAL:HG23  | 2.19                     | 0.43              |
| 39:I:91:GLU:O     | 39:I:93:LEU:N     | 2.52                     | 0.43              |
| 48:R:25:ILE:C     | 48:R:25:ILE:CD1   | 2.88                     | 0.43              |
| 51:U:62:GLU:H     | 51:U:62:GLU:CD    | 2.27                     | 0.43              |
| 52:03:8:MET:HA    | 52:03:11:ILE:HD12 | 2.01                     | 0.43              |
| 53:A:320:A:H2'    | 53:A:321:A:C8     | 2.54                     | 0.43              |
| 53:A:578:C:H2'    | 53:A:579:A:C8     | 2.54                     | 0.43              |
| 53:A:797:C:H2'    | 53:A:798:U:H6     | 1.81                     | 0.43              |
| 54:01:516:C:H2'   | 54:01:517:C:C6    | 2.53                     | 0.43              |
| 54:01:589:U:H2'   | 54:01:590:A:C8    | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:01:799:G:C6    | 54:01:800:A:C6    | 3.06                     | 0.43              |
| 54:01:914:G:H5'   | 54:01:915:C:OP2   | 2.18                     | 0.43              |
| 54:01:1018:U:O2'  | 54:01:1019:U:H5'  | 2.18                     | 0.43              |
| 54:01:2359:C:O2'  | 54:01:2360:G:H5'  | 2.19                     | 0.43              |
| 54:01:2360:G:C2'  | 54:01:2361:G:H5'  | 2.49                     | 0.43              |
| 55:02:13:G:O2'    | 55:02:15:A:H2'    | 2.18                     | 0.43              |
| 55:02:108:A:H5'   | 55:02:109:A:O5'   | 2.19                     | 0.43              |
| 1:04:146:LYS:O    | 1:04:148:GLY:N    | 2.52                     | 0.43              |
| 1:04:181:ARG:CB   | 1:04:181:ARG:HH11 | 2.32                     | 0.43              |
| 1:04:229:HIS:CE1  | 1:04:230:PRO:HD2  | 2.53                     | 0.43              |
| 2:05:68:PHE:O     | 2:05:72:GLY:N     | 2.39                     | 0.43              |
| 3:06:44:ARG:O     | 3:06:45:ALA:HB2   | 2.18                     | 0.43              |
| 7:10:17:GLU:OE2   | 7:10:53:ARG:HG3   | 2.18                     | 0.43              |
| 7:10:28:ALA:HB3   | 7:10:111:ALA:HB2  | 2.00                     | 0.43              |
| 7:10:87:GLU:HB3   | 7:10:93:ALA:HB3   | 2.01                     | 0.43              |
| 9:12:8:PRO:HG3    | 9:12:48:VAL:CG1   | 2.48                     | 0.43              |
| 10:13:76:VAL:H    | 15:18:72:VAL:CG2  | 2.32                     | 0.43              |
| 11:14:14:LYS:O    | 11:14:15:ALA:HB3  | 2.18                     | 0.43              |
| 11:14:58:TYR:CE1  | 11:14:59:ARG:HG3  | 2.54                     | 0.43              |
| 16:19:12:ARG:HH21 | 16:19:12:ARG:HG3  | 1.83                     | 0.43              |
| 16:19:21:LYS:HG2  | 54:01:19:A:H5'    | 2.00                     | 0.43              |
| 16:19:63:ARG:HH11 | 16:19:63:ARG:HG3  | 1.84                     | 0.43              |
| 27:30:24:VAL:CG1  | 27:30:25:THR:H    | 2.28                     | 0.43              |
| 27:30:54:ILE:HG13 | 27:30:56:LYS:HB3  | 2.00                     | 0.43              |
| 33:C:54:ILE:HG13  | 33:C:54:ILE:O     | 2.19                     | 0.43              |
| 33:C:125:ARG:CB   | 33:C:125:ARG:NH1  | 2.82                     | 0.43              |
| 34:D:7:LYS:HZ2    | 34:D:21:LYS:CG    | 2.32                     | 0.43              |
| 34:D:21:LYS:O     | 34:D:21:LYS:HG2   | 2.18                     | 0.43              |
| 36:F:36:ILE:HG13  | 36:F:37:HIS:N     | 2.34                     | 0.43              |
| 36:F:97:THR:HG23  | 36:F:98:GLU:HG2   | 2.00                     | 0.43              |
| 37:G:73:GLU:HG3   | 37:G:74:VAL:N     | 2.33                     | 0.43              |
| 37:G:133:ALA:O    | 37:G:136:LYS:HB3  | 2.19                     | 0.43              |
| 39:I:112:ARG:HE   | 44:N:100:TRP:NE1  | 2.17                     | 0.43              |
| 41:K:49:SER:HA    | 41:K:68:ARG:HH11  | 1.83                     | 0.43              |
| 52:03:43:ASP:O    | 52:03:215:SER:N   | 2.45                     | 0.43              |
| 53:A:26:A:H61     | 53:A:558:G:H1'    | 1.82                     | 0.43              |
| 53:A:273:U:C2'    | 53:A:274:A:H5'    | 2.49                     | 0.43              |
| 53:A:319:G:H2'    | 53:A:320:A:C8     | 2.53                     | 0.43              |
| 53:A:513:C:H2'    | 53:A:514:C:H6     | 1.81                     | 0.43              |
| 53:A:605:U:H2'    | 53:A:606:G:C8     | 2.54                     | 0.43              |
| 54:01:172:A:H2'   | 54:01:173:A:H8    | 1.84                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:01:195:A:H3'   | 54:01:196:A:H4'   | 2.01                     | 0.43              |
| 54:01:315:G:H2'   | 54:01:316:C:O4'   | 2.19                     | 0.43              |
| 54:01:1300:G:C4'  | 54:01:1301:A:C5'  | 2.96                     | 0.43              |
| 54:01:1801:A:H5'' | 54:01:2203:U:H2'  | 1.99                     | 0.43              |
| 54:01:2808:G:H5'  | 54:01:2809:A:OP1  | 2.18                     | 0.43              |
| 58:Y:23:A:H2'     | 58:Y:24:G:H8      | 1.84                     | 0.43              |
| 58:Y:69:G:H2'     | 58:Y:70:G:C8      | 2.53                     | 0.43              |
| 59:Z:150:LYS:HD3  | 59:Z:152:LEU:HD23 | 2.01                     | 0.43              |
| 3:06:82:GLY:O     | 3:06:83:VAL:C     | 2.60                     | 0.43              |
| 4:07:3:LEU:HD23   | 4:07:100:GLU:HG3  | 2.00                     | 0.43              |
| 4:07:7:TYR:HA     | 4:07:11:VAL:HG21  | 2.00                     | 0.43              |
| 8:11:61:TYR:C     | 8:11:63:ASP:N     | 2.76                     | 0.43              |
| 11:14:30:THR:HB   | 11:14:33:ARG:HB3  | 2.01                     | 0.43              |
| 12:15:19:GLY:C    | 12:15:20:LEU:HD12 | 2.43                     | 0.43              |
| 12:15:135:VAL:O   | 12:15:136:MET:OXT | 2.36                     | 0.43              |
| 13:16:37:THR:O    | 13:16:38:LEU:C    | 2.62                     | 0.43              |
| 16:19:44:TYR:O    | 16:19:45:ALA:C    | 2.60                     | 0.43              |
| 19:22:13:ALA:HB1  | 19:22:14:PRO:HD2  | 2.01                     | 0.43              |
| 20:23:5:ARG:O     | 20:23:6:ARG:C     | 2.62                     | 0.43              |
| 24:27:8:GLU:N     | 24:27:8:GLU:OE1   | 2.52                     | 0.43              |
| 25:28:19:HIS:ND1  | 25:28:50:VAL:HG12 | 2.34                     | 0.43              |
| 29:32:14:ARG:HD3  | 54:01:125:A:H5'   | 2.01                     | 0.43              |
| 33:C:35:ASP:OD1   | 33:C:56:ILE:HG13  | 2.19                     | 0.43              |
| 34:D:25:ARG:O     | 34:D:26:ALA:C     | 2.62                     | 0.43              |
| 39:I:35:GLU:HA    | 39:I:39:GLY:HA3   | 2.00                     | 0.43              |
| 41:K:107:THR:O    | 51:U:6:ARG:HG3    | 2.18                     | 0.43              |
| 42:L:109:ARG:HH12 | 53:A:537:G:H5''   | 1.84                     | 0.43              |
| 43:M:105:ALA:HA   | 53:A:948:C:OP1    | 2.19                     | 0.43              |
| 53:A:70:U:H4'     | 53:A:71:A:H8      | 1.84                     | 0.43              |
| 53:A:739:C:H2'    | 53:A:740:U:O4'    | 2.19                     | 0.43              |
| 53:A:1228:C:H2'   | 53:A:1229:A:C8    | 2.53                     | 0.43              |
| 54:01:768:G:N2    | 54:01:1379:U:H1'  | 2.34                     | 0.43              |
| 54:01:935:C:H2'   | 54:01:936:A:H8    | 1.84                     | 0.43              |
| 54:01:1274:A:N1   | 54:01:1302:A:C2   | 2.87                     | 0.43              |
| 54:01:1775:U:H2'  | 54:01:1776:G:H5'  | 2.01                     | 0.43              |
| 1:04:220:ARG:HG3  | 54:01:1789:A:OP1  | 2.18                     | 0.42              |
| 4:07:4:HIS:NE2    | 4:07:8:LYS:HE3    | 2.34                     | 0.42              |
| 6:09:84:ALA:HA    | 6:09:91:PHE:H     | 1.84                     | 0.42              |
| 7:10:118:ILE:N    | 7:10:119:PRO:HD2  | 2.34                     | 0.42              |
| 8:11:104:GLN:O    | 8:11:108:ILE:HG13 | 2.18                     | 0.42              |
| 10:13:35:VAL:HG12 | 10:13:36:GLY:N    | 2.34                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:13:48:PRO:HG3   | 53:A:1422:G:H5'    | 2.00                     | 0.42              |
| 11:14:4:ASN:O      | 54:01:1243:C:H1'   | 2.19                     | 0.42              |
| 11:14:100:ILE:HG13 | 11:14:101:ILE:HG23 | 2.01                     | 0.42              |
| 12:15:44:ARG:HG2   | 12:15:44:ARG:HH21  | 1.83                     | 0.42              |
| 13:16:31:HIS:C     | 13:16:33:ILE:H     | 2.26                     | 0.42              |
| 18:21:59:GLU:OE2   | 18:21:66:ILE:HD11  | 2.18                     | 0.42              |
| 33:C:110:LEU:HG    | 33:C:143:LEU:HD23  | 2.01                     | 0.42              |
| 35:E:160:VAL:O     | 35:E:163:ILE:HG13  | 2.19                     | 0.42              |
| 36:F:46:GLN:HG2    | 36:F:47:LEU:O      | 2.19                     | 0.42              |
| 37:G:89:GLU:CD     | 37:G:89:GLU:N      | 2.77                     | 0.42              |
| 39:I:124:PRO:O     | 39:I:125:GLN:C     | 2.62                     | 0.42              |
| 42:L:6:LEU:HD21    | 42:L:11:ARG:CZ     | 2.49                     | 0.42              |
| 49:S:2:ARG:O       | 49:S:3:SER:CB      | 2.67                     | 0.42              |
| 50:T:16:ALA:HB1    | 50:T:20:ASN:HD21   | 1.84                     | 0.42              |
| 51:U:49:ALA:HA     | 53:A:723:U:C4      | 2.53                     | 0.42              |
| 53:A:815:A:H4'     | 53:A:817:C:C4      | 2.53                     | 0.42              |
| 53:A:925:G:C2      | 53:A:927:G:C8      | 3.06                     | 0.42              |
| 53:A:980:C:H2'     | 53:A:981:U:H5'     | 2.01                     | 0.42              |
| 53:A:1245:C:H2'    | 53:A:1246:A:C8     | 2.54                     | 0.42              |
| 53:A:1429:A:H2'    | 53:A:1430:A:C8     | 2.54                     | 0.42              |
| 54:01:250:G:C6     | 54:01:251:A:C6     | 3.06                     | 0.42              |
| 54:01:414:C:H2'    | 54:01:415:A:H8     | 1.83                     | 0.42              |
| 54:01:445:C:O2'    | 54:01:446:G:H5'    | 2.19                     | 0.42              |
| 54:01:834:G:C2     | 54:01:835:C:C2     | 3.07                     | 0.42              |
| 54:01:1366:A:H2'   | 54:01:1367:A:O4'   | 2.19                     | 0.42              |
| 54:01:1686:C:H2'   | 54:01:1687:G:O4'   | 2.19                     | 0.42              |
| 54:01:1804:C:O2'   | 54:01:1805:A:H5'   | 2.18                     | 0.42              |
| 55:02:51:G:H2'     | 55:02:52:A:O4'     | 2.19                     | 0.42              |
| 57:V:17:U:H2'      | 57:V:18:G:H8       | 1.84                     | 0.42              |
| 1:04:270:ARG:NH1   | 1:04:270:ARG:HB3   | 2.34                     | 0.42              |
| 4:07:103:ILE:HG13  | 4:07:104:THR:N     | 2.34                     | 0.42              |
| 5:08:169:ARG:HH12  | 54:01:1093:G:H5'   | 1.84                     | 0.42              |
| 7:10:67:THR:CG2    | 7:10:74:ASP:HB2    | 2.48                     | 0.42              |
| 8:11:128:ILE:N     | 8:11:128:ILE:CD1   | 2.82                     | 0.42              |
| 9:12:93:ILE:HD11   | 9:12:100:VAL:HG21  | 2.01                     | 0.42              |
| 12:15:20:LEU:HD12  | 12:15:20:LEU:N     | 2.34                     | 0.42              |
| 13:16:2:ARG:HA     | 13:16:5:LYS:HD2    | 2.01                     | 0.42              |
| 13:16:63:ARG:NE    | 54:01:1454:C:H5'   | 2.33                     | 0.42              |
| 16:19:45:ALA:O     | 16:19:49:ARG:HG3   | 2.19                     | 0.42              |
| 16:19:60:TRP:CZ2   | 54:01:995:C:H1'    | 2.54                     | 0.42              |
| 21:24:77:VAL:CG2   | 21:24:78:GLN:N     | 2.82                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:28:4:ILE:O     | 25:28:36:GLU:HA    | 2.19                     | 0.42              |
| 27:30:30:ASP:HB3  | 27:30:34:GLY:H     | 1.84                     | 0.42              |
| 29:32:25:LYS:O    | 29:32:28:ARG:N     | 2.52                     | 0.42              |
| 30:33:6:VAL:O     | 30:33:8:GLY:N      | 2.52                     | 0.42              |
| 32:B:72:LYS:NZ    | 32:B:203:ASP:O     | 2.49                     | 0.42              |
| 32:B:124:THR:O    | 32:B:128:LEU:HD13  | 2.18                     | 0.42              |
| 32:B:162:VAL:CG1  | 32:B:163:ILE:N     | 2.82                     | 0.42              |
| 34:D:191:SER:O    | 34:D:192:ALA:CB    | 2.67                     | 0.42              |
| 37:G:104:VAL:O    | 37:G:107:ALA:HB3   | 2.19                     | 0.42              |
| 42:L:113:ARG:HH11 | 42:L:113:ARG:HG2   | 1.84                     | 0.42              |
| 44:N:20:PHE:O     | 44:N:21:ALA:CB     | 2.67                     | 0.42              |
| 44:N:81:ILE:HG21  | 53:A:1202:U:N3     | 2.34                     | 0.42              |
| 48:R:25:ILE:O     | 48:R:26:ALA:C      | 2.61                     | 0.42              |
| 49:S:73:PHE:C     | 49:S:75:PRO:HD3    | 2.43                     | 0.42              |
| 52:03:180:PHE:HB3 | 52:03:184:LYS:HB2  | 2.01                     | 0.42              |
| 52:03:195:ALA:HA  | 52:03:198:LYS:CD   | 2.45                     | 0.42              |
| 53:A:358:U:H2'    | 53:A:359:G:H8      | 1.84                     | 0.42              |
| 53:A:396:C:H2'    | 53:A:397:A:H5''    | 2.01                     | 0.42              |
| 53:A:428:G:H4'    | 53:A:429:U:O5'     | 2.17                     | 0.42              |
| 53:A:537:G:H2'    | 53:A:538:G:H8      | 1.85                     | 0.42              |
| 53:A:555:U:H2'    | 53:A:556:C:C6      | 2.54                     | 0.42              |
| 53:A:1163:A:H2'   | 53:A:1164:G:H8     | 1.84                     | 0.42              |
| 53:A:1233:G:H2'   | 53:A:1234:C:C6     | 2.53                     | 0.42              |
| 53:A:1484:C:O2'   | 54:01:1961:C:H5'   | 2.19                     | 0.42              |
| 54:01:580:U:O2'   | 54:01:581:C:H5'    | 2.18                     | 0.42              |
| 54:01:1625:C:H2'  | 54:01:1626:A:O4'   | 2.19                     | 0.42              |
| 54:01:2370:G:H2'  | 54:01:2371:G:C8    | 2.54                     | 0.42              |
| 54:01:2372:U:H2'  | 54:01:2373:G:H8    | 1.84                     | 0.42              |
| 56:W:57:A:H2'     | 56:W:58:A:H5'      | 2.02                     | 0.42              |
| 4:07:111:ARG:NH2  | 4:07:112:ASP:OD2   | 2.52                     | 0.42              |
| 5:08:119:GLY:O    | 5:08:120:ILE:HD13  | 2.19                     | 0.42              |
| 8:11:91:LYS:O     | 8:11:95:ASP:OD1    | 2.37                     | 0.42              |
| 9:12:27:ARG:HH21  | 54:01:1142:A:H4'   | 1.84                     | 0.42              |
| 9:12:71:ASP:O     | 9:12:72:LYS:C      | 2.62                     | 0.42              |
| 13:16:35:LYS:HZ2  | 13:16:110:MET:HE1  | 1.84                     | 0.42              |
| 13:16:94:TYR:C    | 13:16:116:VAL:HG23 | 2.44                     | 0.42              |
| 14:17:27:VAL:HG21 | 14:17:40:ILE:HD12  | 2.01                     | 0.42              |
| 15:18:95:LYS:N    | 15:18:95:LYS:CD    | 2.82                     | 0.42              |
| 17:20:1:MET:HB2   | 17:20:43:ASN:ND2   | 2.35                     | 0.42              |
| 19:22:13:ALA:HB1  | 24:27:33:ALA:HB3   | 2.01                     | 0.42              |
| 32:B:6:ARG:HG2    | 32:B:6:ARG:NH1     | 2.33                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:C:14:VAL:HG11  | 33:C:180:ASP:HB2  | 2.01                     | 0.42              |
| 33:C:77:GLY:HA3   | 33:C:82:ASP:OD2   | 2.19                     | 0.42              |
| 34:D:68:GLU:O     | 34:D:69:ARG:C     | 2.62                     | 0.42              |
| 35:E:153:ALA:O    | 35:E:158:LYS:HA   | 2.19                     | 0.42              |
| 36:F:1:MET:SD     | 36:F:66:ALA:HA    | 2.60                     | 0.42              |
| 37:G:142:ARG:HB3  | 56:X:41:C:H4'     | 2.01                     | 0.42              |
| 39:I:101:GLY:C    | 39:I:103:VAL:H    | 2.27                     | 0.42              |
| 40:J:15:HIS:C     | 40:J:17:LEU:N     | 2.75                     | 0.42              |
| 41:K:63:GLN:HG3   | 41:K:98:ALA:HB2   | 2.02                     | 0.42              |
| 41:K:105:ARG:HH11 | 41:K:105:ARG:HG3  | 1.84                     | 0.42              |
| 42:L:39:THR:CG2   | 42:L:40:THR:N     | 2.82                     | 0.42              |
| 42:L:115:LYS:O    | 42:L:116:TYR:HB2  | 2.19                     | 0.42              |
| 47:Q:7:LEU:HD12   | 47:Q:7:LEU:N      | 2.33                     | 0.42              |
| 47:Q:67:SER:C     | 47:Q:69:THR:N     | 2.77                     | 0.42              |
| 48:R:12:PHE:CE2   | 48:R:13:THR:HG22  | 2.54                     | 0.42              |
| 49:S:10:ILE:C     | 49:S:10:ILE:HD12  | 2.44                     | 0.42              |
| 50:T:67:HIS:C     | 50:T:69:ASN:H     | 2.27                     | 0.42              |
| 53:A:210:C:H4'    | 53:A:211:G:C2     | 2.55                     | 0.42              |
| 53:A:709:U:H2'    | 53:A:710:G:H8     | 1.83                     | 0.42              |
| 53:A:1256:A:O2'   | 53:A:1257:A:H5''  | 2.20                     | 0.42              |
| 54:01:633:A:H2'   | 54:01:634:C:C5'   | 2.47                     | 0.42              |
| 54:01:1023:U:O2'  | 54:01:1122:G:H5'  | 2.19                     | 0.42              |
| 54:01:2187:U:H2'  | 54:01:2188:U:C6   | 2.53                     | 0.42              |
| 55:02:55:U:H2'    | 55:02:56:G:H8     | 1.82                     | 0.42              |
| 58:Y:57:G:C2'     | 58:Y:58:A:H5'     | 2.49                     | 0.42              |
| 59:Z:150:LYS:HD3  | 59:Z:152:LEU:HB2  | 2.01                     | 0.42              |
| 2:05:4:LEU:HD22   | 2:05:101:PHE:HE2  | 1.84                     | 0.42              |
| 3:06:176:ASP:OD1  | 3:06:179:SER:HB2  | 2.19                     | 0.42              |
| 6:09:2:GLN:NE2    | 6:09:20:ASN:HB2   | 2.34                     | 0.42              |
| 6:09:4:ILE:HG13   | 6:09:5:LEU:N      | 2.34                     | 0.42              |
| 6:09:41:LYS:O     | 6:09:45:GLU:HG3   | 2.19                     | 0.42              |
| 10:13:25:LEU:O    | 10:13:30:ARG:HD3  | 2.20                     | 0.42              |
| 12:15:12:MET:CA   | 54:01:910:A:H62   | 2.25                     | 0.42              |
| 12:15:63:ILE:HG12 | 12:15:105:MET:HE2 | 2.00                     | 0.42              |
| 24:27:10:SER:O    | 24:27:14:LEU:HB2  | 2.19                     | 0.42              |
| 29:32:3:ARG:HD2   | 29:32:3:ARG:HA    | 1.73                     | 0.42              |
| 33:C:10:ARG:HG2   | 33:C:177:LEU:CD2  | 2.46                     | 0.42              |
| 34:D:96:ARG:HH12  | 34:D:133:SER:HA   | 1.84                     | 0.42              |
| 35:E:59:ILE:HD12  | 35:E:59:ILE:C     | 2.44                     | 0.42              |
| 35:E:149:PRO:HA   | 35:E:152:VAL:CG2  | 2.49                     | 0.42              |
| 44:N:7:ALA:CA     | 44:N:10:VAL:HG12  | 2.48                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:N:8:ARG:CG     | 44:N:12:ARG:HH12  | 2.21                     | 0.42              |
| 45:O:48:ASP:O     | 45:O:49:HIS:C     | 2.62                     | 0.42              |
| 49:S:77:ARG:HD2   | 53:A:960:U:H5     | 1.84                     | 0.42              |
| 51:U:64:ALA:O     | 51:U:66:ARG:N     | 2.52                     | 0.42              |
| 53:A:291:U:H2'    | 53:A:292:G:C8     | 2.54                     | 0.42              |
| 53:A:1432:G:HI1'  | 53:A:1468:A:H62   | 1.83                     | 0.42              |
| 54:01:175:G:H2'   | 54:01:176:A:C8    | 2.53                     | 0.42              |
| 54:01:1101:U:H2'  | 54:01:1102:C:C6   | 2.50                     | 0.42              |
| 54:01:1149:G:H2'  | 54:01:1150:C:C6   | 2.55                     | 0.42              |
| 54:01:1182:G:O2'  | 54:01:1183:U:H5'  | 2.20                     | 0.42              |
| 54:01:1336:A:H2'  | 54:01:1337:G:H8   | 1.84                     | 0.42              |
| 54:01:1370:C:H2'  | 54:01:1371:G:C8   | 2.54                     | 0.42              |
| 2:05:14:ILE:HA    | 15:18:11:GLN:HE22 | 1.84                     | 0.42              |
| 3:06:119:ILE:O    | 3:06:187:VAL:HA   | 2.20                     | 0.42              |
| 3:06:170:ARG:HH21 | 3:06:170:ARG:HG3  | 1.83                     | 0.42              |
| 4:07:72:SER:HB2   | 4:07:80:GLN:N     | 2.35                     | 0.42              |
| 4:07:116:LEU:HD12 | 4:07:116:LEU:N    | 2.34                     | 0.42              |
| 4:07:137:PHE:HA   | 4:07:138:PRO:HD3  | 1.89                     | 0.42              |
| 4:07:172:PHE:HB2  | 4:07:174:PHE:CE2  | 2.54                     | 0.42              |
| 9:12:99:ARG:HA    | 9:12:102:GLU:OE1  | 2.19                     | 0.42              |
| 10:13:109:SER:OG  | 10:13:111:LYS:HG2 | 2.19                     | 0.42              |
| 11:14:19:LEU:N    | 11:14:19:LEU:CD1  | 2.82                     | 0.42              |
| 11:14:41:ARG:NH1  | 54:01:807:U:OP2   | 2.52                     | 0.42              |
| 14:17:76:LYS:O    | 14:17:80:GLU:HG3  | 2.18                     | 0.42              |
| 16:19:43:GLN:HE21 | 17:20:77:PHE:HB3  | 1.85                     | 0.42              |
| 19:22:12:ARG:O    | 19:22:13:ALA:HB2  | 2.19                     | 0.42              |
| 20:23:11:ILE:HG13 | 20:23:20:LYS:O    | 2.18                     | 0.42              |
| 21:24:80:HIS:ND1  | 21:24:81:PRO:HD2  | 2.35                     | 0.42              |
| 25:28:4:ILE:HG13  | 25:28:58:GLU:HA   | 2.02                     | 0.42              |
| 25:28:11:SER:OG   | 54:01:989:G:OP2   | 2.30                     | 0.42              |
| 34:D:32:LYS:HE3   | 53:A:413:G:C6     | 2.54                     | 0.42              |
| 40:J:8:ILE:HB     | 40:J:74:VAL:HB    | 2.02                     | 0.42              |
| 41:K:24:ALA:CB    | 41:K:29:THR:HG22  | 2.49                     | 0.42              |
| 42:L:40:THR:HA    | 42:L:41:PRO:HD3   | 1.90                     | 0.42              |
| 43:M:14:ALA:O     | 43:M:15:VAL:C     | 2.62                     | 0.42              |
| 47:Q:45:VAL:CG2   | 47:Q:60:ILE:HD13  | 2.43                     | 0.42              |
| 47:Q:64:ARG:HB3   | 47:Q:64:ARG:NH1   | 2.35                     | 0.42              |
| 50:T:17:ARG:NH2   | 50:T:18:LYS:NZ    | 2.67                     | 0.42              |
| 51:U:39:LYS:O     | 51:U:40:PRO:C     | 2.61                     | 0.42              |
| 53:A:31:G:N2      | 53:A:47:C:H5''    | 2.35                     | 0.42              |
| 53:A:259:G:O2'    | 53:A:260:G:H5'    | 2.19                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 53:A:1449:C:O2'    | 53:A:1450:U:H5'   | 2.20                     | 0.42              |
| 54:01:889:C:H2'    | 54:01:890:C:O4'   | 2.20                     | 0.42              |
| 54:01:1019:U:H3    | 54:01:1142:A:H62  | 1.67                     | 0.42              |
| 54:01:2011:U:H2'   | 54:01:2012:G:O4'  | 2.20                     | 0.42              |
| 54:01:2070:A:H2'   | 54:01:2071:A:C8   | 2.55                     | 0.42              |
| 54:01:2869:G:H2'   | 54:01:2870:C:C6   | 2.55                     | 0.42              |
| 58:Y:23:A:H2'      | 58:Y:24:G:C8      | 2.54                     | 0.42              |
| 1:04:270:ARG:HH11  | 1:04:270:ARG:HB2  | 1.84                     | 0.42              |
| 7:10:41:LEU:O      | 7:10:44:ALA:HB3   | 2.20                     | 0.42              |
| 7:10:54:VAL:HA     | 7:10:84:TYR:O     | 2.19                     | 0.42              |
| 7:10:122:GLN:HB3   | 7:10:123:ILE:H    | 1.68                     | 0.42              |
| 9:12:43:GLU:O      | 9:12:44:TYR:C     | 2.63                     | 0.42              |
| 12:15:78:LEU:HD23  | 12:15:79:ALA:HB2  | 2.01                     | 0.42              |
| 13:16:103:ARG:HH11 | 54:01:1287:A:H5'  | 1.84                     | 0.42              |
| 18:21:14:ALA:O     | 18:21:18:ARG:HG3  | 2.20                     | 0.42              |
| 20:23:50:ALA:O     | 20:23:52:ASN:N    | 2.46                     | 0.42              |
| 24:27:52:ARG:HB2   | 24:27:52:ARG:CZ   | 2.50                     | 0.42              |
| 25:28:43:ILE:O     | 25:28:47:ILE:HG13 | 2.19                     | 0.42              |
| 29:32:35:ARG:O     | 29:32:38:GLY:N    | 2.50                     | 0.42              |
| 30:33:63:TYR:CE2   | 54:01:242:G:H5''  | 2.53                     | 0.42              |
| 34:D:34:GLU:O      | 34:D:35:GLN:HG2   | 2.19                     | 0.42              |
| 42:L:7:VAL:HG11    | 47:Q:37:ILE:HD11  | 2.00                     | 0.42              |
| 42:L:20:VAL:HG23   | 42:L:20:VAL:O     | 2.19                     | 0.42              |
| 44:N:43:ALA:C      | 44:N:45:LEU:N     | 2.76                     | 0.42              |
| 46:P:76:LYS:HZ3    | 53:A:473:U:H5''   | 1.85                     | 0.42              |
| 53:A:834:U:H2'     | 53:A:835:U:C6     | 2.55                     | 0.42              |
| 54:01:18:U:H2'     | 54:01:19:A:C8     | 2.55                     | 0.42              |
| 54:01:288:U:H2'    | 54:01:289:G:C8    | 2.54                     | 0.42              |
| 54:01:386:G:H3'    | 54:01:387:U:C5'   | 2.49                     | 0.42              |
| 54:01:955:U:H3     | 54:01:962:G:H1    | 1.68                     | 0.42              |
| 54:01:2236:U:H2'   | 54:01:2237:G:O4'  | 2.20                     | 0.42              |
| 54:01:2297:A:N6    | 54:01:2319:G:H1'  | 2.35                     | 0.42              |
| 54:01:2345:G:N3    | 54:01:2381:A:H2'  | 2.33                     | 0.42              |
| 54:01:2364:C:H2'   | 54:01:2365:G:O4'  | 2.19                     | 0.42              |
| 59:Z:120:PHE:HB2   | 59:Z:131:LEU:HB2  | 2.01                     | 0.42              |
| 2:05:124:ARG:NH1   | 2:05:163:GLY:HA3  | 2.34                     | 0.42              |
| 3:06:122:GLU:HG3   | 3:06:123:LYS:N    | 2.35                     | 0.42              |
| 3:06:164:LEU:HD23  | 3:06:167:VAL:HG21 | 2.02                     | 0.42              |
| 3:06:189:THR:O     | 3:06:193:VAL:HG23 | 2.19                     | 0.42              |
| 5:08:86:LEU:HG     | 5:08:163:TYR:HD1  | 1.83                     | 0.42              |
| 8:11:10:LEU:O      | 8:11:56:VAL:HG12  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:12:109:LEU:HD23 | 9:12:109:LEU:HA   | 1.89                     | 0.42              |
| 10:13:48:PRO:HB3  | 53:A:1422:G:H4'   | 2.02                     | 0.42              |
| 10:13:70:ARG:HG2  | 10:13:70:ARG:HH11 | 1.85                     | 0.42              |
| 16:19:35:PHE:CZ   | 16:19:39:ILE:HD11 | 2.55                     | 0.42              |
| 16:19:94:LEU:O    | 16:19:97:ILE:HB   | 2.20                     | 0.42              |
| 18:21:52:GLU:HA   | 18:21:55:ILE:HD12 | 2.00                     | 0.42              |
| 36:F:20:GLY:HA2   | 36:F:23:GLU:CD    | 2.44                     | 0.42              |
| 36:F:79:ARG:HG2   | 36:F:79:ARG:NH1   | 2.35                     | 0.42              |
| 37:G:104:VAL:O    | 37:G:108:ARG:HG2  | 2.20                     | 0.42              |
| 47:Q:39:ARG:HG3   | 47:Q:39:ARG:NH1   | 2.35                     | 0.42              |
| 47:Q:69:THR:HG22  | 47:Q:70:LYS:N     | 2.21                     | 0.42              |
| 48:R:19:GLU:O     | 48:R:20:ILE:C     | 2.61                     | 0.42              |
| 53:A:54:C:H2'     | 53:A:352:C:H41    | 1.83                     | 0.42              |
| 53:A:231:U:H2'    | 53:A:232:G:H8     | 1.84                     | 0.42              |
| 53:A:309:A:H2'    | 53:A:310:G:H8     | 1.85                     | 0.42              |
| 53:A:314:C:H2'    | 53:A:315:A:C8     | 2.54                     | 0.42              |
| 53:A:1411:C:H2'   | 53:A:1412:C:C6    | 2.54                     | 0.42              |
| 54:01:1105:U:H2'  | 54:01:1106:G:C5'  | 2.48                     | 0.42              |
| 54:01:1362:C:H2'  | 54:01:1363:C:O4'  | 2.20                     | 0.42              |
| 54:01:1423:G:H2'  | 54:01:1424:G:C8   | 2.53                     | 0.42              |
| 54:01:1949:G:H2'  | 54:01:1950:G:C8   | 2.54                     | 0.42              |
| 54:01:2673:G:H2'  | 54:01:2674:G:C8   | 2.54                     | 0.42              |
| 55:02:10:G:H2'    | 55:02:11:C:O4'    | 2.19                     | 0.42              |
| 1:04:89:ASN:N     | 1:04:89:ASN:ND2   | 2.67                     | 0.42              |
| 1:04:179:GLU:HG2  | 54:01:1799:G:C8   | 2.55                     | 0.42              |
| 2:05:22:ILE:HA    | 2:05:23:PRO:HD3   | 1.85                     | 0.42              |
| 4:07:149:ARG:HB2  | 4:07:149:ARG:CZ   | 2.50                     | 0.42              |
| 5:08:1:SER:C      | 5:08:3:VAL:H      | 2.27                     | 0.42              |
| 6:09:64:ALA:O     | 6:09:67:ALA:HB3   | 2.19                     | 0.42              |
| 6:09:132:PHE:O    | 6:09:140:ALA:N    | 2.45                     | 0.42              |
| 7:10:58:THR:O     | 7:10:59:LEU:C     | 2.63                     | 0.42              |
| 8:11:100:ILE:CG2  | 8:11:101:SER:H    | 2.26                     | 0.42              |
| 9:12:117:ALA:HA   | 9:12:120:ARG:HH22 | 1.82                     | 0.42              |
| 11:14:14:LYS:HA   | 11:14:14:LYS:CE   | 2.41                     | 0.42              |
| 15:18:83:ILE:O    | 15:18:84:SER:C    | 2.62                     | 0.42              |
| 16:19:24:TYR:HB3  | 54:01:533:G:OP1   | 2.20                     | 0.42              |
| 17:20:74:ILE:N    | 17:20:74:ILE:CD1  | 2.80                     | 0.42              |
| 19:22:6:ARG:HG3   | 19:22:6:ARG:HH11  | 1.85                     | 0.42              |
| 21:24:60:VAL:C    | 21:24:61:LEU:HD12 | 2.44                     | 0.42              |
| 27:30:18:HIS:C    | 27:30:20:ALA:N    | 2.78                     | 0.42              |
| 31:34:19:ARG:HD2  | 31:34:24:ARG:CD   | 2.50                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:D:144:ILE:N    | 34:D:144:ILE:CD1   | 2.82                     | 0.42              |
| 34:D:145:ARG:HD2  | 34:D:147:LYS:HZ1   | 1.84                     | 0.42              |
| 35:E:87:VAL:O     | 35:E:87:VAL:HG13   | 2.20                     | 0.42              |
| 37:G:31:VAL:HG22  | 37:G:32:ASP:N      | 2.34                     | 0.42              |
| 38:H:77:VAL:HG21  | 38:H:127:TYR:CE2   | 2.55                     | 0.42              |
| 45:O:86:LEU:HD12  | 45:O:87:ARG:N      | 2.35                     | 0.42              |
| 47:Q:28:VAL:CG2   | 47:Q:29:LYS:N      | 2.82                     | 0.42              |
| 50:T:42:ASP:HB3   | 50:T:45:ALA:HB3    | 2.02                     | 0.42              |
| 52:03:63:THR:HG21 | 52:03:192:LEU:HD13 | 2.02                     | 0.42              |
| 53:A:82:G:H1      | 53:A:87:C:N4       | 2.18                     | 0.42              |
| 53:A:295:C:H2'    | 53:A:296:U:O4'     | 2.20                     | 0.42              |
| 53:A:594:U:O2'    | 53:A:595:A:H5'     | 2.20                     | 0.42              |
| 53:A:956:U:O2'    | 53:A:957:U:H5'     | 2.20                     | 0.42              |
| 53:A:1238:A:H2'   | 53:A:1238:A:N3     | 2.34                     | 0.42              |
| 53:A:1435:G:H2'   | 53:A:1436:U:C6     | 2.55                     | 0.42              |
| 54:01:799:G:N1    | 54:01:800:A:N6     | 2.68                     | 0.42              |
| 54:01:819:A:C4    | 54:01:1189:A:C2    | 3.07                     | 0.42              |
| 54:01:839:U:H2'   | 54:01:840:C:C6     | 2.55                     | 0.42              |
| 54:01:1704:C:H2'  | 54:01:1705:A:H8    | 1.84                     | 0.42              |
| 54:01:1770:G:C6   | 54:01:1983:G:C6    | 3.08                     | 0.42              |
| 54:01:2026:U:H2'  | 54:01:2027:G:C8    | 2.55                     | 0.42              |
| 54:01:2811:G:O2'  | 54:01:2812:G:H5'   | 2.20                     | 0.42              |
| 1:04:131:MET:HE1  | 1:04:183:VAL:CG2   | 2.49                     | 0.42              |
| 4:07:107:VAL:O    | 4:07:110:ILE:HG13  | 2.19                     | 0.42              |
| 6:09:135:HIS:O    | 6:09:136:SER:C     | 2.62                     | 0.42              |
| 8:11:100:ILE:CG2  | 8:11:101:SER:N     | 2.83                     | 0.42              |
| 9:12:34:ARG:NH2   | 16:19:69:ARG:HD2   | 2.35                     | 0.42              |
| 13:16:117:ASP:O   | 13:16:118:ARG:HB2  | 2.20                     | 0.42              |
| 14:17:74:VAL:O    | 14:17:78:VAL:HG23  | 2.20                     | 0.42              |
| 23:26:40:GLU:OE2  | 23:26:43:LYS:HG2   | 2.20                     | 0.42              |
| 27:30:24:VAL:CG1  | 27:30:25:THR:N     | 2.82                     | 0.42              |
| 44:N:53:ASP:HA    | 44:N:58:ARG:CD     | 2.50                     | 0.42              |
| 47:Q:56:ASP:HB2   | 47:Q:79:GLU:O      | 2.20                     | 0.42              |
| 50:T:77:ASN:O     | 50:T:81:GLN:HG2    | 2.20                     | 0.42              |
| 53:A:56:U:H2'     | 53:A:57:G:C8       | 2.55                     | 0.42              |
| 53:A:635:A:H2'    | 53:A:636:U:C6      | 2.55                     | 0.42              |
| 53:A:746:A:H2'    | 53:A:747:A:C8      | 2.55                     | 0.42              |
| 53:A:1346:A:O2'   | 53:A:1347:G:H4'    | 2.20                     | 0.42              |
| 54:01:306:U:H2'   | 54:01:307:G:O4'    | 2.19                     | 0.42              |
| 54:01:578:G:H21   | 54:01:1252:G:N2    | 2.17                     | 0.42              |
| 54:01:1182:G:H2'  | 54:01:1183:U:O4'   | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:01:1507:C:H2'  | 54:01:1508:A:C4'  | 2.50                     | 0.42              |
| 54:01:1542:U:H2'  | 54:01:1543:G:O4'  | 2.20                     | 0.42              |
| 54:01:2478:A:H2'  | 54:01:2479:U:O4'  | 2.20                     | 0.42              |
| 55:02:79:G:O2'    | 55:02:80:U:H5'    | 2.20                     | 0.42              |
| 2:05:98:VAL:O     | 2:05:98:VAL:HG22  | 2.20                     | 0.42              |
| 4:07:103:ILE:HG22 | 4:07:174:PHE:CZ   | 2.55                     | 0.42              |
| 7:10:59:LEU:O     | 7:10:63:ALA:N     | 2.52                     | 0.42              |
| 9:12:57:LEU:C     | 9:12:57:LEU:HD12  | 2.45                     | 0.42              |
| 9:12:81:ILE:HG23  | 9:12:82:GLY:H     | 1.83                     | 0.42              |
| 10:13:22:ILE:HG12 | 10:13:41:ILE:HA   | 2.02                     | 0.42              |
| 18:21:96:ILE:HG13 | 18:21:96:ILE:O    | 2.20                     | 0.42              |
| 19:22:12:ARG:HB2  | 19:22:33:LYS:O    | 2.20                     | 0.42              |
| 19:22:34:VAL:HG11 | 19:22:43:ILE:HD13 | 2.01                     | 0.42              |
| 24:27:42:LEU:O    | 24:27:43:LEU:C    | 2.63                     | 0.42              |
| 24:27:49:ASP:O    | 24:27:53:VAL:HG23 | 2.20                     | 0.42              |
| 25:28:24:LEU:HD23 | 25:28:24:LEU:C    | 2.45                     | 0.42              |
| 28:31:8:ILE:HD11  | 28:31:33:LEU:HD12 | 2.02                     | 0.42              |
| 28:31:8:ILE:HD12  | 28:31:50:GLU:HG2  | 2.01                     | 0.42              |
| 32:B:15:PHE:O     | 59:Z:43:LYS:NZ    | 2.32                     | 0.42              |
| 32:B:131:LYS:O    | 32:B:132:GLU:C    | 2.63                     | 0.42              |
| 32:B:164:ASP:O    | 32:B:168:GLU:HG2  | 2.20                     | 0.42              |
| 33:C:2:GLN:HB2    | 53:A:1190:G:O2'   | 2.20                     | 0.42              |
| 34:D:13:ARG:NH2   | 53:A:543:U:H5'    | 2.34                     | 0.42              |
| 34:D:97:LEU:HD23  | 34:D:117:VAL:HG11 | 2.02                     | 0.42              |
| 34:D:138:PRO:HA   | 34:D:181:PHE:CD2  | 2.55                     | 0.42              |
| 35:E:160:VAL:HG13 | 35:E:161:GLU:H    | 1.85                     | 0.42              |
| 37:G:142:ARG:HH11 | 37:G:142:ARG:HG3  | 1.84                     | 0.42              |
| 39:I:29:ILE:O     | 39:I:29:ILE:HG23  | 2.20                     | 0.42              |
| 41:K:109:ILE:HD13 | 51:U:16:ARG:HH11  | 1.84                     | 0.42              |
| 43:M:6:ILE:O      | 43:M:7:ASN:C      | 2.62                     | 0.42              |
| 50:T:30:PHE:O     | 50:T:33:LYS:HB3   | 2.19                     | 0.42              |
| 50:T:73:ARG:O     | 50:T:76:ALA:HB3   | 2.20                     | 0.42              |
| 53:A:24:U:H2'     | 53:A:25:C:H6      | 1.84                     | 0.42              |
| 53:A:33:A:H2'     | 53:A:34:C:H6      | 1.85                     | 0.42              |
| 53:A:1001:C:H2'   | 53:A:1002:G:C8    | 2.55                     | 0.42              |
| 53:A:1002:G:H2'   | 53:A:1003:G:O4'   | 2.19                     | 0.42              |
| 53:A:1352:C:H2'   | 53:A:1353:G:H8    | 1.85                     | 0.42              |
| 53:A:1496:C:H2'   | 53:A:1497:G:O4'   | 2.20                     | 0.42              |
| 54:01:35:G:O2'    | 54:01:36:G:H5'    | 2.20                     | 0.42              |
| 54:01:1368:G:H2'  | 54:01:1369:G:C8   | 2.50                     | 0.42              |
| 54:01:2194:U:H2'  | 54:01:2195:U:C6   | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:01:2292:U:H2'  | 54:01:2293:G:H8   | 1.84                     | 0.42              |
| 56:X:67:C:H2'     | 56:X:68:C:C6      | 2.55                     | 0.42              |
| 8:11:96:LYS:HD2   | 8:11:96:LYS:N     | 2.35                     | 0.41              |
| 15:18:87:ARG:HB3  | 15:18:87:ARG:NH1  | 2.34                     | 0.41              |
| 30:33:34:LYS:HE2  | 30:33:34:LYS:HB3  | 1.90                     | 0.41              |
| 33:C:2:GLN:HG3    | 33:C:3:LYS:H      | 1.85                     | 0.41              |
| 35:E:93:VAL:HG21  | 35:E:138:ALA:HB3  | 2.00                     | 0.41              |
| 37:G:144:ALA:O    | 37:G:145:GLU:C    | 2.62                     | 0.41              |
| 46:P:6:LEU:HD22   | 46:P:17:TYR:HB3   | 2.01                     | 0.41              |
| 47:Q:51:GLU:O     | 47:Q:77:VAL:HG21  | 2.20                     | 0.41              |
| 53:A:88:U:H2'     | 53:A:89:U:C6      | 2.55                     | 0.41              |
| 53:A:222:C:H2'    | 53:A:223:A:H8     | 1.85                     | 0.41              |
| 53:A:1074:G:O2'   | 53:A:1075:U:H5'   | 2.20                     | 0.41              |
| 53:A:1148:U:H2'   | 53:A:1149:C:O4'   | 2.20                     | 0.41              |
| 53:A:1193:G:O2'   | 53:A:1194:U:H5'   | 2.20                     | 0.41              |
| 54:01:340:A:H2'   | 54:01:341:C:O4'   | 2.20                     | 0.41              |
| 54:01:403:U:O3'   | 54:01:404:A:H4'   | 2.20                     | 0.41              |
| 54:01:940:G:C3'   | 54:01:941:A:H5''  | 2.50                     | 0.41              |
| 54:01:1844:C:H2'  | 54:01:1845:G:C8   | 2.55                     | 0.41              |
| 56:W:23:C:H2'     | 56:W:24:U:C6      | 2.55                     | 0.41              |
| 2:05:62:LYS:HB2   | 2:05:63:PRO:HD3   | 2.03                     | 0.41              |
| 2:05:129:THR:HG22 | 2:05:130:GLN:O    | 2.20                     | 0.41              |
| 3:06:69:ARG:HH11  | 54:01:674:G:H1'   | 1.86                     | 0.41              |
| 3:06:148:ILE:HD13 | 3:06:187:VAL:HG11 | 2.02                     | 0.41              |
| 4:07:39:VAL:HG22  | 4:07:41:GLU:H     | 1.85                     | 0.41              |
| 4:07:74:ALA:O     | 4:07:75:GLY:C     | 2.63                     | 0.41              |
| 4:07:102:LEU:HD12 | 4:07:106:ALA:CB   | 2.50                     | 0.41              |
| 5:08:137:LYS:HA   | 5:08:140:ILE:CD1  | 2.50                     | 0.41              |
| 6:09:4:ILE:HG22   | 6:09:37:VAL:O     | 2.20                     | 0.41              |
| 7:10:77:VAL:O     | 7:10:77:VAL:HG12  | 2.20                     | 0.41              |
| 10:13:20:MET:O    | 10:13:42:THR:HG22 | 2.20                     | 0.41              |
| 11:14:90:VAL:HG12 | 11:14:91:ASP:N    | 2.35                     | 0.41              |
| 33:C:34:SER:O     | 33:C:37:LYS:HB2   | 2.20                     | 0.41              |
| 34:D:190:LEU:O    | 34:D:191:SER:C    | 2.63                     | 0.41              |
| 35:E:113:VAL:HG13 | 35:E:114:LEU:N    | 2.36                     | 0.41              |
| 37:G:22:LEU:O     | 37:G:26:VAL:HG23  | 2.20                     | 0.41              |
| 40:J:44:THR:HG23  | 40:J:69:THR:C     | 2.44                     | 0.41              |
| 42:L:20:VAL:C     | 42:L:22:ALA:N     | 2.78                     | 0.41              |
| 46:P:5:ARG:HB2    | 53:A:376:G:H5''   | 2.02                     | 0.41              |
| 47:Q:28:VAL:HG22  | 47:Q:29:LYS:H     | 1.84                     | 0.41              |
| 48:R:54:LEU:O     | 48:R:58:ILE:HG12  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 51:U:17:ARG:HG2  | 51:U:21:SER:HB2   | 2.01                     | 0.41              |
| 53:A:373:A:H2'   | 53:A:374:A:H8     | 1.86                     | 0.41              |
| 54:01:326:G:H2'  | 54:01:327:G:C8    | 2.55                     | 0.41              |
| 54:01:443:A:H2'  | 54:01:443:A:N3    | 2.35                     | 0.41              |
| 54:01:950:G:H2'  | 54:01:951:C:C6    | 2.55                     | 0.41              |
| 54:01:1318:U:H2' | 54:01:1319:C:C6   | 2.54                     | 0.41              |
| 54:01:1749:A:H2' | 54:01:1750:G:H8   | 1.86                     | 0.41              |
| 54:01:1827:U:H2' | 54:01:1828:G:O4'  | 2.20                     | 0.41              |
| 54:01:1996:C:O2  | 54:01:1997:C:H1'  | 2.20                     | 0.41              |
| 54:01:2049:G:O2' | 54:01:2050:C:H5'  | 2.21                     | 0.41              |
| 1:04:83:ASP:HB2  | 1:04:90:ILE:HD13  | 2.02                     | 0.41              |
| 3:06:64:GLY:O    | 3:06:65:THR:C     | 2.64                     | 0.41              |
| 4:07:141:ASP:CB  | 4:07:144:LYS:HD3  | 2.51                     | 0.41              |
| 5:08:44:HIS:CG   | 5:08:45:ALA:N     | 2.88                     | 0.41              |
| 6:09:4:ILE:CG2   | 6:09:37:VAL:HB    | 2.51                     | 0.41              |
| 6:09:9:VAL:HG11  | 6:09:12:LEU:HD11  | 2.01                     | 0.41              |
| 13:16:48:VAL:O   | 13:16:51:LEU:HB2  | 2.19                     | 0.41              |
| 19:22:6:ARG:O    | 19:22:10:VAL:HG23 | 2.19                     | 0.41              |
| 19:22:51:PHE:C   | 19:22:52:GLU:HG2  | 2.46                     | 0.41              |
| 33:C:107:LYS:HA  | 33:C:108:PRO:HD2  | 1.89                     | 0.41              |
| 34:D:25:ARG:HH12 | 34:D:30:LYS:NZ    | 2.18                     | 0.41              |
| 34:D:196:GLU:H   | 34:D:196:GLU:CD   | 2.28                     | 0.41              |
| 35:E:52:ALA:HB3  | 35:E:58:ALA:CB    | 2.50                     | 0.41              |
| 38:H:3:GLN:OE1   | 38:H:3:GLN:HA     | 2.20                     | 0.41              |
| 53:A:66:A:H5'    | 53:A:173:U:O4     | 2.20                     | 0.41              |
| 53:A:225:C:H2'   | 53:A:226:G:C5'    | 2.45                     | 0.41              |
| 53:A:871:U:H5''  | 53:A:872:A:OP2    | 2.20                     | 0.41              |
| 54:01:6:A:H2'    | 54:01:7:G:C8      | 2.55                     | 0.41              |
| 54:01:74:A:H4'   | 54:01:75:G:O5'    | 2.20                     | 0.41              |
| 54:01:191:A:H2'  | 54:01:192:C:C6    | 2.54                     | 0.41              |
| 54:01:1697:G:H4' | 54:01:1978:A:H5'' | 2.01                     | 0.41              |
| 54:01:2636:C:H2' | 54:01:2637:U:H6   | 1.86                     | 0.41              |
| 54:01:2889:C:H2' | 54:01:2890:G:O4'  | 2.20                     | 0.41              |
| 56:X:21:A:H61    | 56:X:47:U:H5'     | 1.85                     | 0.41              |
| 59:Z:62:ILE:C    | 59:Z:62:ILE:HD12  | 2.45                     | 0.41              |
| 1:04:18:VAL:HG23 | 1:04:202:ARG:HB2  | 2.01                     | 0.41              |
| 1:04:209:ALA:HA  | 1:04:212:TRP:CZ2  | 2.54                     | 0.41              |
| 1:04:270:ARG:CB  | 1:04:270:ARG:HH11 | 2.34                     | 0.41              |
| 3:06:29:HIS:NE2  | 11:14:8:PRO:HD3   | 2.35                     | 0.41              |
| 5:08:29:ASN:HB3  | 5:08:78:VAL:HA    | 2.01                     | 0.41              |
| 6:09:1:MET:HE3   | 6:09:3:VAL:HG23   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:09:24:GLY:O     | 6:09:25:TYR:C      | 2.63                     | 0.41              |
| 11:14:79:LEU:H    | 11:14:113:ALA:HB3  | 1.85                     | 0.41              |
| 13:16:20:MET:HG3  | 13:16:21:PHE:N     | 2.35                     | 0.41              |
| 13:16:36:THR:OG1  | 13:16:37:THR:N     | 2.51                     | 0.41              |
| 20:23:9:GLU:OE2   | 20:23:21:ARG:HB3   | 2.20                     | 0.41              |
| 23:26:38:TRP:HB2  | 23:26:45:PHE:CE1   | 2.55                     | 0.41              |
| 24:27:16:THR:HA   | 24:27:19:LEU:HD12  | 2.02                     | 0.41              |
| 24:27:51:ALA:O    | 24:27:52:ARG:C     | 2.62                     | 0.41              |
| 29:32:17:GLY:O    | 29:32:18:PHE:C     | 2.63                     | 0.41              |
| 32:B:102:ASN:HD21 | 32:B:105:THR:HB    | 1.86                     | 0.41              |
| 33:C:151:GLU:HB2  | 33:C:166:TRP:HB3   | 2.03                     | 0.41              |
| 35:E:82:HIS:CD2   | 38:H:95:MET:HE2    | 2.55                     | 0.41              |
| 38:H:90:GLU:O     | 38:H:91:LEU:C      | 2.62                     | 0.41              |
| 39:I:23:GLY:N     | 39:I:60:LEU:HA     | 2.35                     | 0.41              |
| 39:I:57:VAL:HG12  | 39:I:58:GLU:N      | 2.35                     | 0.41              |
| 41:K:78:ILE:HG22  | 41:K:79:LYS:N      | 2.35                     | 0.41              |
| 41:K:85:VAL:HG23  | 41:K:111:ASP:OD1   | 2.21                     | 0.41              |
| 42:L:29:LYS:HA    | 53:A:363:A:OP1     | 2.20                     | 0.41              |
| 43:M:49:GLU:C     | 43:M:51:GLN:H      | 2.29                     | 0.41              |
| 44:N:2:LYS:C      | 44:N:4:SER:N       | 2.78                     | 0.41              |
| 47:Q:4:ILE:C      | 47:Q:4:ILE:CD1     | 2.94                     | 0.41              |
| 49:S:33:TRP:O     | 49:S:35:ARG:HG3    | 2.20                     | 0.41              |
| 53:A:629:A:H2'    | 53:A:630:A:O4'     | 2.21                     | 0.41              |
| 54:01:464:U:C2    | 54:01:788:A:C6     | 3.08                     | 0.41              |
| 54:01:776:G:H1    | 54:01:2072:C:C5'   | 2.34                     | 0.41              |
| 54:01:802:A:H2'   | 54:01:802:A:N3     | 2.35                     | 0.41              |
| 54:01:1537:G:N3   | 54:01:1537:G:H3'   | 2.35                     | 0.41              |
| 54:01:2366:A:H2'  | 54:01:2367:G:O4'   | 2.20                     | 0.41              |
| 56:X:13:C:C3'     | 56:X:14:A:H5''     | 2.50                     | 0.41              |
| 58:Y:57:G:H2'     | 58:Y:58:A:H5'      | 2.02                     | 0.41              |
| 58:Y:69:G:H2'     | 58:Y:70:G:H8       | 1.86                     | 0.41              |
| 2:05:148:GLN:O    | 54:01:2052:A:H4'   | 2.20                     | 0.41              |
| 6:09:7:ASP:CG     | 6:09:8:LYS:N       | 2.78                     | 0.41              |
| 6:09:25:TYR:CD2   | 6:09:30:LEU:HD11   | 2.55                     | 0.41              |
| 10:13:105:ARG:C   | 10:13:107:LEU:N    | 2.77                     | 0.41              |
| 12:15:60:GLN:HG3  | 12:15:108:VAL:HG12 | 2.03                     | 0.41              |
| 16:19:31:TYR:C    | 16:19:33:VAL:H     | 2.28                     | 0.41              |
| 16:19:113:LYS:O   | 16:19:116:LEU:HB3  | 2.20                     | 0.41              |
| 17:20:6:GLN:HG2   | 17:20:11:GLN:HG3   | 2.01                     | 0.41              |
| 17:20:72:VAL:O    | 17:20:74:ILE:HD12  | 2.20                     | 0.41              |
| 19:22:51:PHE:O    | 19:22:52:GLU:C     | 2.63                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:23:86:PHE:CZ   | 20:23:91:LYS:HE2   | 2.54                     | 0.41              |
| 29:32:12:ARG:HG3  | 29:32:12:ARG:NH2   | 2.35                     | 0.41              |
| 37:G:91:ARG:HB3   | 37:G:92:PRO:HD2    | 2.02                     | 0.41              |
| 38:H:13:ILE:O     | 38:H:17:GLN:HG2    | 2.21                     | 0.41              |
| 43:M:66:GLY:O     | 43:M:69:ARG:N      | 2.54                     | 0.41              |
| 44:N:86:ALA:HB3   | 44:N:92:ILE:HD11   | 2.02                     | 0.41              |
| 45:O:58:MET:HA    | 45:O:61:GLN:HB3    | 2.03                     | 0.41              |
| 46:P:20:VAL:HG21  | 46:P:32:PHE:HB2    | 2.02                     | 0.41              |
| 53:A:829:G:O2'    | 53:A:830:G:H5'     | 2.20                     | 0.41              |
| 53:A:1245:C:H2'   | 53:A:1246:A:H8     | 1.85                     | 0.41              |
| 53:A:1504:G:OP1   | 53:A:1507:A:H4'    | 2.20                     | 0.41              |
| 54:01:82:U:H2'    | 54:01:83:A:O4'     | 2.20                     | 0.41              |
| 54:01:226:A:H2'   | 54:01:227:A:C8     | 2.55                     | 0.41              |
| 54:01:593:U:H2'   | 54:01:594:U:C6     | 2.56                     | 0.41              |
| 54:01:1316:U:H2'  | 54:01:1317:G:C8    | 2.56                     | 0.41              |
| 54:01:1526:C:H2'  | 54:01:1527:G:O4'   | 2.21                     | 0.41              |
| 54:01:1965:C:H3'  | 54:01:1966:A:C8    | 2.55                     | 0.41              |
| 54:01:2830:C:O2'  | 54:01:2831:G:H5'   | 2.20                     | 0.41              |
| 55:02:88:C:H5''   | 55:02:89:U:OP1     | 2.20                     | 0.41              |
| 1:04:20:ASN:HA    | 1:04:21:PRO:HD2    | 1.93                     | 0.41              |
| 4:07:149:ARG:NH1  | 4:07:149:ARG:CB    | 2.84                     | 0.41              |
| 6:09:3:VAL:HA     | 6:09:39:ALA:HB3    | 2.02                     | 0.41              |
| 7:10:88:HIS:O     | 7:10:90:GLY:N      | 2.53                     | 0.41              |
| 11:14:23:ILE:N    | 11:14:23:ILE:CD1   | 2.79                     | 0.41              |
| 11:14:118:THR:O   | 11:14:120:VAL:N    | 2.53                     | 0.41              |
| 12:15:83:GLY:HA2  | 54:01:2276:G:P     | 2.61                     | 0.41              |
| 13:16:79:LEU:C    | 13:16:81:ASN:H     | 2.28                     | 0.41              |
| 20:23:102:ILE:OXT | 20:23:102:ILE:HG22 | 2.20                     | 0.41              |
| 33:C:125:ARG:HB2  | 33:C:125:ARG:NH1   | 2.33                     | 0.41              |
| 38:H:28:SER:OG    | 38:H:29:SER:N      | 2.53                     | 0.41              |
| 40:J:25:ILE:O     | 40:J:29:ALA:HB2    | 2.20                     | 0.41              |
| 53:A:314:C:O2'    | 53:A:315:A:H5'     | 2.20                     | 0.41              |
| 53:A:634:C:H2'    | 53:A:635:A:C8      | 2.56                     | 0.41              |
| 54:01:259:G:O2'   | 54:01:260:G:H5'    | 2.20                     | 0.41              |
| 54:01:1435:G:H2'  | 54:01:1436:G:C8    | 2.55                     | 0.41              |
| 54:01:1935:G:O2'  | 54:01:1936:A:H5'   | 2.21                     | 0.41              |
| 54:01:2087:G:H2'  | 54:01:2088:A:H8    | 1.86                     | 0.41              |
| 1:04:176:ARG:HG2  | 54:01:1820:U:OP1   | 2.21                     | 0.41              |
| 3:06:148:ILE:O    | 3:06:169:VAL:HA    | 2.21                     | 0.41              |
| 4:07:166:ARG:O    | 4:07:170:ALA:N     | 2.53                     | 0.41              |
| 8:11:75:ALA:HA    | 8:11:78:LEU:HD12   | 2.02                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 17:20:74:ILE:HB    | 17:20:87:GLN:O    | 2.20                     | 0.41              |
| 17:20:93:PHE:CD1   | 17:20:93:PHE:C    | 2.98                     | 0.41              |
| 19:22:58:VAL:C     | 19:22:59:ASN:HD22 | 2.29                     | 0.41              |
| 19:22:73:ARG:NH1   | 54:01:456:C:H2'   | 2.35                     | 0.41              |
| 23:26:17:ARG:HH11  | 23:26:17:ARG:HG3  | 1.85                     | 0.41              |
| 23:26:30:PRO:O     | 23:26:32:LEU:HG   | 2.21                     | 0.41              |
| 34:D:197:HIS:HE1   | 35:E:103:GLY:HA2  | 1.86                     | 0.41              |
| 46:P:11:ALA:HA     | 53:A:44:A:OP1     | 2.20                     | 0.41              |
| 49:S:54:ARG:HB3    | 53:A:958:A:C2     | 2.56                     | 0.41              |
| 53:A:151:A:H2'     | 53:A:152:A:O4'    | 2.21                     | 0.41              |
| 54:01:279:A:C2'    | 54:01:280:U:H5'   | 2.50                     | 0.41              |
| 54:01:570:G:O2'    | 54:01:571:U:H5'   | 2.21                     | 0.41              |
| 54:01:898:C:H2'    | 54:01:899:A:O4'   | 2.19                     | 0.41              |
| 54:01:1313:U:H2'   | 54:01:1610:A:C2   | 2.55                     | 0.41              |
| 54:01:2315:G:H2'   | 54:01:2316:G:H8   | 1.85                     | 0.41              |
| 54:01:2810:A:H2'   | 54:01:2811:G:O4'  | 2.20                     | 0.41              |
| 1:04:243:PRO:O     | 1:04:251:THR:HG22 | 2.21                     | 0.41              |
| 1:04:266:ILE:HG21  | 1:04:269:ARG:CD   | 2.46                     | 0.41              |
| 4:07:103:ILE:HG22  | 4:07:174:PHE:HE1  | 1.84                     | 0.41              |
| 11:14:50:PHE:CE2   | 11:14:52:GLY:HA2  | 2.56                     | 0.41              |
| 13:16:14:SER:O     | 13:16:15:SER:C    | 2.64                     | 0.41              |
| 13:16:103:ARG:HH22 | 13:16:110:MET:HE3 | 1.85                     | 0.41              |
| 15:18:96:LEU:O     | 15:18:97:TYR:C    | 2.64                     | 0.41              |
| 16:19:42:GLY:O     | 16:19:45:ALA:HB3  | 2.21                     | 0.41              |
| 18:21:42:LYS:CB    | 54:01:2010:G:H5'' | 2.45                     | 0.41              |
| 33:C:113:LYS:H     | 33:C:184:ASN:ND2  | 2.19                     | 0.41              |
| 36:F:66:ALA:CB     | 36:F:67:PRO:HD2   | 2.42                     | 0.41              |
| 38:H:90:GLU:O      | 38:H:90:GLU:CG    | 2.68                     | 0.41              |
| 40:J:50:THR:HG23   | 40:J:64:GLN:HG2   | 2.03                     | 0.41              |
| 43:M:25:GLY:N      | 53:A:1329:A:H5''  | 2.31                     | 0.41              |
| 43:M:33:LEU:HD23   | 43:M:40:GLU:HA    | 2.03                     | 0.41              |
| 45:O:31:LEU:O      | 45:O:35:ILE:HG13  | 2.21                     | 0.41              |
| 46:P:33:ILE:N      | 46:P:33:ILE:CD1   | 2.81                     | 0.41              |
| 48:R:56:ARG:O      | 48:R:60:ARG:HG3   | 2.21                     | 0.41              |
| 53:A:162:A:H2'     | 53:A:163:C:O4'    | 2.21                     | 0.41              |
| 53:A:1139:G:H5''   | 53:A:1140:C:H5    | 1.85                     | 0.41              |
| 53:A:1270:G:H2'    | 53:A:1271:A:H8    | 1.86                     | 0.41              |
| 53:A:1326:U:H2'    | 53:A:1327:C:C6    | 2.55                     | 0.41              |
| 53:A:1363:A:O2'    | 53:A:1364:U:H2'   | 2.21                     | 0.41              |
| 53:A:1453:G:H3'    | 53:A:1453:G:N3    | 2.36                     | 0.41              |
| 53:A:1489:G:O2'    | 53:A:1490:U:H5'   | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:01:395:U:H2'    | 54:01:396:G:H8     | 1.86                     | 0.41              |
| 54:01:1787:A:H2'   | 54:01:1787:A:N3    | 2.35                     | 0.41              |
| 54:01:2747:G:O6    | 54:01:2755:C:H5''  | 2.21                     | 0.41              |
| 2:05:125:TRP:CD1   | 2:05:160:LYS:HB3   | 2.56                     | 0.41              |
| 2:05:151:THR:HB    | 54:01:2571:U:O2'   | 2.21                     | 0.41              |
| 3:06:48:THR:C      | 3:06:50:ALA:H      | 2.29                     | 0.41              |
| 3:06:118:LEU:O     | 3:06:119:ILE:HD13  | 2.21                     | 0.41              |
| 3:06:178:VAL:CG1   | 3:06:179:SER:N     | 2.82                     | 0.41              |
| 3:06:196:VAL:O     | 3:06:199:MET:HB3   | 2.21                     | 0.41              |
| 4:07:21:TYR:CD1    | 4:07:26:GLN:NE2    | 2.89                     | 0.41              |
| 4:07:139:GLU:CD    | 4:07:139:GLU:N     | 2.79                     | 0.41              |
| 4:07:141:ASP:C     | 4:07:143:ASP:N     | 2.79                     | 0.41              |
| 5:08:70:LEU:O      | 5:08:74:MET:HG3    | 2.20                     | 0.41              |
| 6:09:125:THR:HA    | 6:09:146:VAL:HB    | 2.02                     | 0.41              |
| 7:10:118:ILE:N     | 7:10:119:PRO:CD    | 2.84                     | 0.41              |
| 9:12:101:ILE:HB    | 9:12:124:VAL:HG11  | 2.03                     | 0.41              |
| 10:13:6:THR:HG23   | 54:01:1666:G:O3'   | 2.21                     | 0.41              |
| 10:13:21:CYS:CA    | 10:13:41:ILE:HG22  | 2.47                     | 0.41              |
| 11:14:103:ILE:CD1  | 54:01:259:G:H4'    | 2.51                     | 0.41              |
| 12:15:4:PRO:HG2    | 12:15:70:ASP:HA    | 2.03                     | 0.41              |
| 12:15:36:VAL:HB    | 12:15:127:LYS:O    | 2.21                     | 0.41              |
| 12:15:102:LEU:HD13 | 12:15:124:LEU:HD13 | 2.03                     | 0.41              |
| 13:16:2:ARG:CB     | 13:16:5:LYS:HD2    | 2.51                     | 0.41              |
| 13:16:69:ARG:C     | 13:16:71:ARG:H     | 2.29                     | 0.41              |
| 14:17:94:ARG:NH2   | 14:17:94:ARG:CB    | 2.84                     | 0.41              |
| 18:21:9:HIS:H      | 18:21:102:HIS:CE1  | 2.39                     | 0.41              |
| 23:26:13:THR:HG21  | 54:01:188:G:H5'    | 2.03                     | 0.41              |
| 24:27:9:LYS:HG2    | 24:27:10:SER:N     | 2.36                     | 0.41              |
| 28:31:10:LEU:HD23  | 28:31:50:GLU:HA    | 2.03                     | 0.41              |
| 31:34:4:ARG:C      | 31:34:6:SER:N      | 2.77                     | 0.41              |
| 32:B:15:PHE:O      | 59:Z:43:LYS:CG     | 2.69                     | 0.41              |
| 32:B:22:TRP:CZ3    | 32:B:24:PRO:HA     | 2.56                     | 0.41              |
| 32:B:46:VAL:N      | 32:B:47:PRO:HD2    | 2.36                     | 0.41              |
| 33:C:126:ARG:HG2   | 33:C:126:ARG:NH1   | 2.35                     | 0.41              |
| 34:D:131:ILE:HG22  | 34:D:133:SER:N     | 2.34                     | 0.41              |
| 34:D:133:SER:O     | 34:D:134:TYR:C     | 2.64                     | 0.41              |
| 35:E:148:SER:HB2   | 35:E:149:PRO:CD    | 2.44                     | 0.41              |
| 36:F:12:PRO:O      | 36:F:15:SER:CB     | 2.66                     | 0.41              |
| 36:F:75:GLU:O      | 36:F:78:PHE:HB2    | 2.21                     | 0.41              |
| 38:H:35:ILE:O      | 38:H:39:LEU:HG     | 2.21                     | 0.41              |
| 38:H:120:LEU:HD12  | 38:H:120:LEU:C     | 2.45                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:I:38:PHE:HA    | 39:I:41:GLU:OE1   | 2.20                     | 0.41              |
| 39:I:82:ILE:O     | 39:I:86:LEU:HG    | 2.21                     | 0.41              |
| 40:J:10:LEU:HD12  | 40:J:10:LEU:C     | 2.45                     | 0.41              |
| 41:K:28:ASN:CG    | 41:K:29:THR:N     | 2.79                     | 0.41              |
| 42:L:22:ALA:O     | 42:L:23:LEU:CB    | 2.69                     | 0.41              |
| 42:L:58:ASN:OD1   | 42:L:60:PHE:N     | 2.51                     | 0.41              |
| 42:L:73:LEU:H     | 42:L:73:LEU:CD1   | 2.34                     | 0.41              |
| 45:O:25:GLU:O     | 45:O:26:VAL:C     | 2.64                     | 0.41              |
| 48:R:71:ASP:OD1   | 48:R:72:ARG:N     | 2.53                     | 0.41              |
| 52:O3:26:ALA:HB1  | 52:O3:214:ILE:CD1 | 2.47                     | 0.41              |
| 52:O3:166:ASP:OD2 | 52:O3:168:ASN:HB2 | 2.20                     | 0.41              |
| 53:A:536:C:H2'    | 53:A:537:G:C8     | 2.56                     | 0.41              |
| 53:A:594:U:H2'    | 53:A:595:A:O4'    | 2.21                     | 0.41              |
| 53:A:605:U:H2'    | 53:A:606:G:H8     | 1.86                     | 0.41              |
| 53:A:729:A:O2'    | 53:A:730:G:H5'    | 2.21                     | 0.41              |
| 53:A:1157:A:C2    | 53:A:1181:G:C4    | 3.09                     | 0.41              |
| 53:A:1158:C:H3'   | 53:A:1158:C:O2    | 2.21                     | 0.41              |
| 53:A:1171:A:H2'   | 53:A:1172:C:H6    | 1.86                     | 0.41              |
| 53:A:1186:G:O2'   | 53:A:1187:G:H5'   | 2.21                     | 0.41              |
| 53:A:1471:U:O2'   | 53:A:1472:U:H5'   | 2.20                     | 0.41              |
| 54:O1:27:G:C2     | 54:O1:512:G:N3    | 2.89                     | 0.41              |
| 54:O1:881:G:O2'   | 54:O1:882:G:H5'   | 2.21                     | 0.41              |
| 54:O1:983:A:N6    | 54:O1:984:A:C2    | 2.88                     | 0.41              |
| 54:O1:1103:A:H2'  | 54:O1:1104:C:OP1  | 2.21                     | 0.41              |
| 54:O1:1128:G:C6   | 54:O1:2518:A:C6   | 3.09                     | 0.41              |
| 54:O1:1378:A:H1'  | 54:O1:1379:U:C5   | 2.56                     | 0.41              |
| 54:O1:1458:U:H4'  | 54:O1:1459:G:C4   | 2.56                     | 0.41              |
| 54:O1:1501:G:O2'  | 54:O1:1502:A:H5'  | 2.21                     | 0.41              |
| 54:O1:1844:C:H2'  | 54:O1:1845:G:H8   | 1.85                     | 0.41              |
| 54:O1:2134:A:O2'  | 54:O1:2159:G:H1'  | 2.21                     | 0.41              |
| 54:O1:2317:A:H2'  | 54:O1:2318:G:O4'  | 2.21                     | 0.41              |
| 54:O1:2421:G:H2'  | 56:X:76:A:N6      | 2.36                     | 0.41              |
| 54:O1:2743:U:H2'  | 54:O1:2744:G:C5'  | 2.48                     | 0.41              |
| 56:W:63:G:H2'     | 56:W:64:G:H8      | 1.84                     | 0.41              |
| 2:O5:151:THR:CB   | 2:O5:152:PRO:HD3  | 2.30                     | 0.41              |
| 3:O6:118:LEU:HD11 | 3:O6:188:MET:SD   | 2.61                     | 0.41              |
| 4:O7:102:LEU:HD12 | 4:O7:106:ALA:HB3  | 2.03                     | 0.41              |
| 5:O8:93:TYR:CD1   | 5:O8:106:LEU:HA   | 2.56                     | 0.41              |
| 6:O9:77:THR:HG23  | 6:O9:77:THR:O     | 2.21                     | 0.41              |
| 6:O9:132:PHE:CB   | 6:O9:140:ALA:HB3  | 2.47                     | 0.41              |
| 8:11:4:VAL:HG13   | 8:11:7:TYR:CE2    | 2.55                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:14:78:ARG:NH2   | 54:01:626:A:H2'   | 2.36                     | 0.41              |
| 11:14:111:ILE:N    | 11:14:111:ILE:CD1 | 2.75                     | 0.41              |
| 14:17:94:ARG:O     | 14:17:95:SER:C    | 2.63                     | 0.41              |
| 20:23:85:ARG:HD3   | 20:23:87:GLU:CD   | 2.46                     | 0.41              |
| 25:28:11:SER:OG    | 25:28:13:ILE:HG13 | 2.21                     | 0.41              |
| 26:29:26:SER:OG    | 26:29:27:THR:N    | 2.53                     | 0.41              |
| 27:30:39:ARG:HG2   | 27:30:39:ARG:NH2  | 2.36                     | 0.41              |
| 32:B:21:TYR:O      | 32:B:189:ASN:HB2  | 2.21                     | 0.41              |
| 32:B:25:LYS:HD2    | 32:B:191:ASP:CG   | 2.45                     | 0.41              |
| 33:C:89:VAL:O      | 33:C:93:ILE:HG13  | 2.21                     | 0.41              |
| 34:D:173:ASP:C     | 34:D:175:GLY:N    | 2.79                     | 0.41              |
| 35:E:155:LYS:HE2   | 38:H:70:VAL:HG13  | 2.03                     | 0.41              |
| 40:J:7:ARG:HG2     | 40:J:7:ARG:HH11   | 1.85                     | 0.41              |
| 41:K:84:MET:HA     | 41:K:110:THR:O    | 2.20                     | 0.41              |
| 43:M:113:LYS:H     | 43:M:114:PRO:CD   | 2.17                     | 0.41              |
| 52:03:15:VAL:CG2   | 52:03:33:LEU:HD21 | 2.49                     | 0.41              |
| 52:03:170:ILE:HG21 | 54:01:2177:C:H1'  | 2.03                     | 0.41              |
| 53:A:1441:A:H62    | 53:A:1461:G:H21   | 1.68                     | 0.41              |
| 54:01:164:C:H2'    | 54:01:165:A:O4'   | 2.21                     | 0.41              |
| 54:01:443:A:H5''   | 54:01:444:C:H5''  | 2.03                     | 0.41              |
| 54:01:629:G:H5''   | 54:01:650:C:O2'   | 2.20                     | 0.41              |
| 54:01:1326:U:H5'   | 54:01:2011:U:H1'  | 2.02                     | 0.41              |
| 54:01:2070:A:H2'   | 54:01:2071:A:O4'  | 2.20                     | 0.41              |
| 54:01:2671:G:H2'   | 54:01:2672:U:C6   | 2.56                     | 0.41              |
| 1:04:64:VAL:HG21   | 1:04:86:ARG:HH21  | 1.85                     | 0.40              |
| 7:10:56:ARG:H      | 54:01:1084:A:C4'  | 2.34                     | 0.40              |
| 8:11:27:LEU:O      | 8:11:32:VAL:HB    | 2.21                     | 0.40              |
| 8:11:74:PRO:HB3    | 54:01:1059:G:O3'  | 2.21                     | 0.40              |
| 11:14:91:ASP:HA    | 11:14:123:ARG:O   | 2.20                     | 0.40              |
| 14:17:51:ALA:HB2   | 14:17:81:ARG:HD2  | 2.02                     | 0.40              |
| 16:19:108:LEU:CA   | 17:20:48:LYS:HZ3  | 2.29                     | 0.40              |
| 18:21:86:MET:HB2   | 18:21:96:ILE:HD13 | 2.03                     | 0.40              |
| 24:27:19:LEU:HD22  | 24:27:23:ARG:HE   | 1.86                     | 0.40              |
| 30:33:23:HIS:HD2   | 30:33:49:VAL:HG22 | 1.86                     | 0.40              |
| 32:B:75:ALA:HB1    | 32:B:209:VAL:HG11 | 2.03                     | 0.40              |
| 35:E:15:ILE:N      | 35:E:15:ILE:CD1   | 2.82                     | 0.40              |
| 35:E:55:VAL:N      | 35:E:56:PRO:HD2   | 2.36                     | 0.40              |
| 37:G:75:LYS:NZ     | 37:G:77:ARG:HD3   | 2.36                     | 0.40              |
| 39:I:49:GLN:HB2    | 39:I:50:PRO:CD    | 2.51                     | 0.40              |
| 40:J:41:PRO:CB     | 53:A:1151:A:H1'   | 2.52                     | 0.40              |
| 40:J:57:VAL:HG13   | 40:J:58:ASN:N     | 2.36                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:N:40:ARG:HH22  | 49:S:6:LYS:CD     | 2.27                     | 0.40              |
| 49:S:65:MET:HG2   | 49:S:73:PHE:HZ    | 1.86                     | 0.40              |
| 50:T:35:TYR:HA    | 50:T:38:ILE:HD12  | 2.03                     | 0.40              |
| 50:T:73:ARG:HB2   | 50:T:73:ARG:HH11  | 1.86                     | 0.40              |
| 53:A:232:G:O2'    | 53:A:233:C:H5'    | 2.22                     | 0.40              |
| 53:A:1342:C:H2'   | 53:A:1343:G:C8    | 2.57                     | 0.40              |
| 54:01:7:G:H2'     | 54:01:8:C:H6      | 1.86                     | 0.40              |
| 54:01:353:C:H2'   | 54:01:354:A:H8    | 1.86                     | 0.40              |
| 54:01:381:G:H2'   | 54:01:382:A:C8    | 2.55                     | 0.40              |
| 54:01:859:G:H2'   | 54:01:860:U:OP2   | 2.20                     | 0.40              |
| 54:01:1857:G:H1'  | 54:01:1885:A:N6   | 2.36                     | 0.40              |
| 54:01:2619:C:O2'  | 54:01:2620:C:H5'  | 2.21                     | 0.40              |
| 54:01:2742:G:O2'  | 54:01:2743:U:H5'  | 2.21                     | 0.40              |
| 56:X:31:G:H2'     | 56:X:32:C:H5'     | 2.03                     | 0.40              |
| 59:Z:97:THR:O     | 59:Z:97:THR:HG22  | 2.21                     | 0.40              |
| 1:04:104:LEU:HD11 | 1:04:155:ARG:HG2  | 2.03                     | 0.40              |
| 2:05:18:ASP:OD1   | 2:05:20:VAL:HG23  | 2.22                     | 0.40              |
| 2:05:123:LYS:NZ   | 54:01:2724:U:H5'' | 2.35                     | 0.40              |
| 4:07:28:PRO:HB2   | 4:07:168:LEU:HD22 | 2.02                     | 0.40              |
| 9:12:29:ALA:O     | 9:12:32:LEU:HB2   | 2.21                     | 0.40              |
| 9:12:113:PRO:HD2  | 54:01:558:U:P     | 2.61                     | 0.40              |
| 12:15:2:LEU:HD12  | 12:15:2:LEU:N     | 2.36                     | 0.40              |
| 12:15:12:MET:SD   | 12:15:72:PRO:HD2  | 2.61                     | 0.40              |
| 13:16:69:ARG:HH21 | 13:16:69:ARG:HG3  | 1.86                     | 0.40              |
| 14:17:33:ARG:O    | 14:17:34:HIS:HB2  | 2.21                     | 0.40              |
| 15:18:12:MET:HE3  | 15:18:76:HIS:HE2  | 1.83                     | 0.40              |
| 22:25:16:ARG:HG3  | 54:01:2271:G:H5'  | 2.03                     | 0.40              |
| 28:31:12:SER:HA   | 28:31:48:TYR:CD1  | 2.56                     | 0.40              |
| 31:34:25:VAL:HB   | 31:34:35:GLN:HG2  | 2.04                     | 0.40              |
| 34:D:62:ARG:HG3   | 34:D:62:ARG:NH1   | 2.35                     | 0.40              |
| 36:F:18:VAL:HB    | 36:F:19:PRO:HD3   | 2.02                     | 0.40              |
| 37:G:134:VAL:O    | 37:G:138:GLU:HG2  | 2.21                     | 0.40              |
| 39:I:46:VAL:HA    | 39:I:49:GLN:CG    | 2.51                     | 0.40              |
| 44:N:21:ALA:H     | 44:N:24:ALA:HB2   | 1.85                     | 0.40              |
| 44:N:41:TRP:O     | 44:N:45:LEU:HB2   | 2.20                     | 0.40              |
| 46:P:74:LEU:O     | 46:P:78:VAL:HG12  | 2.21                     | 0.40              |
| 51:U:34:ARG:HD3   | 51:U:34:ARG:HA    | 1.90                     | 0.40              |
| 53:A:40:C:H2'     | 53:A:41:G:C8      | 2.55                     | 0.40              |
| 53:A:701:U:H5''   | 53:A:703:G:H1'    | 2.02                     | 0.40              |
| 53:A:757:U:H4'    | 53:A:822:U:O2     | 2.21                     | 0.40              |
| 53:A:815:A:H4'    | 53:A:817:C:C5     | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:01:924:G:H2'   | 54:01:925:A:C8    | 2.56                     | 0.40              |
| 54:01:1183:U:H2'  | 54:01:1184:U:C6   | 2.56                     | 0.40              |
| 54:01:1361:G:H2'  | 54:01:1362:C:C6   | 2.56                     | 0.40              |
| 54:01:1672:A:N6   | 54:01:1673:G:C6   | 2.89                     | 0.40              |
| 54:01:1979:U:H2'  | 54:01:1980:G:H8   | 1.86                     | 0.40              |
| 54:01:2097:A:H2'  | 54:01:2098:U:O4'  | 2.21                     | 0.40              |
| 54:01:2715:C:H2'  | 54:01:2716:C:C5'  | 2.50                     | 0.40              |
| 1:04:118:GLY:N    | 1:04:128:THR:O    | 2.54                     | 0.40              |
| 1:04:221:GLY:HA2  | 1:04:224:MET:HE3  | 2.02                     | 0.40              |
| 1:04:226:PRO:HD3  | 1:04:233:GLY:HA2  | 2.02                     | 0.40              |
| 3:06:94:GLN:NE2   | 54:01:660:C:H4'   | 2.36                     | 0.40              |
| 3:06:171:ASP:O    | 3:06:172:ALA:C    | 2.65                     | 0.40              |
| 5:08:53:PRO:HG3   | 5:08:61:TRP:CD2   | 2.57                     | 0.40              |
| 12:15:77:PRO:O    | 12:15:78:LEU:C    | 2.65                     | 0.40              |
| 14:17:110:ALA:HB1 | 14:17:117:PHE:HE2 | 1.85                     | 0.40              |
| 15:18:85:VAL:HG12 | 15:18:86:LYS:N    | 2.35                     | 0.40              |
| 16:19:5:ARG:HG3   | 16:19:5:ARG:O     | 2.21                     | 0.40              |
| 16:19:93:ILE:O    | 16:19:94:LEU:C    | 2.64                     | 0.40              |
| 19:22:73:ARG:HH12 | 54:01:456:C:H2'   | 1.87                     | 0.40              |
| 32:B:206:ILE:HG13 | 59:Z:45:GLU:OE1   | 2.22                     | 0.40              |
| 33:C:72:PRO:O     | 33:C:73:GLY:C     | 2.64                     | 0.40              |
| 34:D:119:HIS:CG   | 53:A:438:U:H4'    | 2.56                     | 0.40              |
| 35:E:96:GLN:HG2   | 35:E:97:PRO:CD    | 2.48                     | 0.40              |
| 36:F:42:TRP:HB2   | 36:F:59:TYR:HB2   | 2.02                     | 0.40              |
| 36:F:88:MET:SD    | 48:R:63:TYR:HD2   | 2.44                     | 0.40              |
| 38:H:113:ARG:HG2  | 38:H:113:ARG:HH11 | 1.86                     | 0.40              |
| 39:I:88:GLU:N     | 39:I:88:GLU:OE1   | 2.51                     | 0.40              |
| 39:I:95:SER:C     | 39:I:97:LEU:N     | 2.78                     | 0.40              |
| 40:J:42:LEU:HB3   | 40:J:43:PRO:HD2   | 2.02                     | 0.40              |
| 42:L:115:LYS:C    | 42:L:117:GLY:H    | 2.29                     | 0.40              |
| 43:M:89:ARG:NH2   | 43:M:94:LEU:HB3   | 2.36                     | 0.40              |
| 45:O:86:LEU:HD12  | 45:O:87:ARG:HB2   | 2.02                     | 0.40              |
| 47:Q:12:VAL:HB    | 47:Q:21:VAL:HG13  | 2.03                     | 0.40              |
| 49:S:57:VAL:HA    | 49:S:58:PRO:HD3   | 1.92                     | 0.40              |
| 52:03:53:ARG:HD3  | 56:X:61:C:O2'     | 2.22                     | 0.40              |
| 53:A:113:G:H2'    | 53:A:114:U:C6     | 2.56                     | 0.40              |
| 53:A:537:G:H2'    | 53:A:538:G:C8     | 2.56                     | 0.40              |
| 53:A:1289:A:H2'   | 53:A:1290:G:H5'   | 2.02                     | 0.40              |
| 54:01:532:A:H2'   | 54:01:532:A:N3    | 2.37                     | 0.40              |
| 54:01:845:A:H61   | 54:01:932:U:H3    | 1.70                     | 0.40              |
| 54:01:1952:A:N6   | 54:01:1953:A:N1   | 2.69                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:01:2339:C:H2'  | 54:01:2340:A:C8   | 2.56                     | 0.40              |
| 55:02:118:C:H2'   | 55:02:119:A:C8    | 2.56                     | 0.40              |
| 1:04:250:GLN:HB3  | 1:04:254:LYS:HG2  | 2.03                     | 0.40              |
| 2:05:33:ARG:O     | 2:05:33:ARG:HG3   | 2.22                     | 0.40              |
| 2:05:166:GLY:C    | 2:05:168:GLU:N    | 2.76                     | 0.40              |
| 3:06:7:ASP:CG     | 3:06:8:ALA:N      | 2.76                     | 0.40              |
| 3:06:33:VAL:O     | 3:06:34:ALA:C     | 2.65                     | 0.40              |
| 3:06:57:LYS:HB2   | 54:01:797:G:OP2   | 2.22                     | 0.40              |
| 3:06:115:GLN:C    | 3:06:117:ARG:N    | 2.79                     | 0.40              |
| 4:07:76:PHE:O     | 4:07:77:LYS:HB2   | 2.21                     | 0.40              |
| 4:07:115:GLY:HA2  | 4:07:175:PRO:HB2  | 2.04                     | 0.40              |
| 6:09:76:GLU:C     | 6:09:142:VAL:HG13 | 2.46                     | 0.40              |
| 7:10:117:LEU:O    | 7:10:118:ILE:HB   | 2.22                     | 0.40              |
| 9:12:69:ARG:HH11  | 9:12:69:ARG:HG3   | 1.86                     | 0.40              |
| 10:13:22:ILE:HB   | 54:01:1952:A:C2   | 2.56                     | 0.40              |
| 11:14:20:GLY:O    | 11:14:21:ARG:HD3  | 2.21                     | 0.40              |
| 11:14:33:ARG:HD2  | 11:14:39:LYS:O    | 2.22                     | 0.40              |
| 12:15:78:LEU:HD23 | 12:15:79:ALA:CB   | 2.51                     | 0.40              |
| 14:17:74:VAL:O    | 14:17:75:GLY:C    | 2.65                     | 0.40              |
| 15:18:38:ARG:CG   | 15:18:39:LEU:N    | 2.83                     | 0.40              |
| 18:21:17:VAL:HG12 | 18:21:76:VAL:HG21 | 2.03                     | 0.40              |
| 32:B:72:LYS:O     | 32:B:76:SER:N     | 2.55                     | 0.40              |
| 33:C:5:HIS:CG     | 44:N:88:MET:HB3   | 2.56                     | 0.40              |
| 33:C:69:THR:OG1   | 33:C:70:ALA:N     | 2.55                     | 0.40              |
| 34:D:186:GLU:O    | 34:D:189:ASP:HB2  | 2.22                     | 0.40              |
| 35:E:108:GLY:O    | 35:E:109:ALA:CB   | 2.70                     | 0.40              |
| 36:F:13:ASP:C     | 36:F:15:SER:N     | 2.80                     | 0.40              |
| 37:G:31:VAL:C     | 37:G:33:GLY:N     | 2.80                     | 0.40              |
| 37:G:110:ARG:O    | 37:G:110:ARG:HG2  | 2.20                     | 0.40              |
| 40:J:89:ARG:HG2   | 40:J:89:ARG:HH11  | 1.85                     | 0.40              |
| 43:M:27:THR:CG2   | 53:A:1328:C:H5''  | 2.49                     | 0.40              |
| 44:N:18:LYS:HE3   | 44:N:19:TYR:CZ    | 2.57                     | 0.40              |
| 45:O:27:GLN:O     | 45:O:30:LEU:HB3   | 2.22                     | 0.40              |
| 46:P:35:ARG:HG3   | 46:P:35:ARG:O     | 2.21                     | 0.40              |
| 47:Q:58:VAL:HA    | 47:Q:78:VAL:HG22  | 2.03                     | 0.40              |
| 49:S:36:ARG:H     | 49:S:36:ARG:HG2   | 1.70                     | 0.40              |
| 53:A:578:C:H2'    | 53:A:579:A:H8     | 1.85                     | 0.40              |
| 54:01:128:C:H2'   | 54:01:129:C:C6    | 2.56                     | 0.40              |
| 54:01:527:C:H4'   | 54:01:528:A:O4'   | 2.22                     | 0.40              |
| 54:01:1106:G:H5'  | 54:01:1106:G:H8   | 1.87                     | 0.40              |
| 54:01:1336:A:H2'  | 54:01:1337:G:C8   | 2.57                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:01:1350:C:C2'  | 54:01:1351:C:H5'  | 2.52                     | 0.40              |
| 54:01:1475:G:O2'  | 54:01:1476:U:C6   | 2.72                     | 0.40              |
| 54:01:1509:A:H2'  | 54:01:1510:G:C8   | 2.56                     | 0.40              |
| 54:01:1538:G:O2'  | 54:01:1539:U:H5'  | 2.22                     | 0.40              |
| 54:01:1603:A:H2'  | 54:01:1603:A:N3   | 2.37                     | 0.40              |
| 54:01:1655:A:H2'  | 54:01:1656:C:O4'  | 2.21                     | 0.40              |
| 54:01:1900:A:C2   | 54:01:1970:A:C6   | 3.09                     | 0.40              |
| 54:01:2204:G:H2'  | 54:01:2205:A:C8   | 2.56                     | 0.40              |
| 54:01:2240:U:O2'  | 54:01:2241:A:H5'  | 2.21                     | 0.40              |
| 54:01:2692:G:O2'  | 54:01:2693:G:H5'  | 2.21                     | 0.40              |
| 54:01:2788:C:H2'  | 54:01:2789:C:C6   | 2.55                     | 0.40              |
| 1:04:153:LEU:HD13 | 1:04:175:LEU:CD2  | 2.48                     | 0.40              |
| 3:06:83:VAL:O     | 3:06:85:PHE:N     | 2.54                     | 0.40              |
| 4:07:154:THR:HG21 | 54:01:2314:A:O4'  | 2.22                     | 0.40              |
| 9:12:81:ILE:HD11  | 54:01:2514:U:H4'  | 2.04                     | 0.40              |
| 11:14:9:ALA:HB3   | 11:14:12:SER:HB2  | 2.03                     | 0.40              |
| 12:15:44:ARG:HG2  | 12:15:44:ARG:NH2  | 2.36                     | 0.40              |
| 17:20:49:ILE:HD12 | 17:20:51:VAL:C    | 2.45                     | 0.40              |
| 18:21:89:ALA:O    | 18:21:91:GLY:N    | 2.54                     | 0.40              |
| 20:23:86:PHE:O    | 20:23:88:ASP:O    | 2.40                     | 0.40              |
| 31:34:27:CYS:SG   | 31:34:30:GLU:N    | 2.95                     | 0.40              |
| 32:B:53:LEU:HD23  | 32:B:56:LEU:HD12  | 2.02                     | 0.40              |
| 34:D:137:SER:O    | 34:D:140:ASP:OD2  | 2.40                     | 0.40              |
| 35:E:104:ILE:HG23 | 35:E:104:ILE:O    | 2.21                     | 0.40              |
| 36:F:3:HIS:H      | 36:F:92:THR:HG22  | 1.83                     | 0.40              |
| 38:H:4:ASP:HA     | 38:H:5:PRO:HD2    | 1.94                     | 0.40              |
| 40:J:80:THR:HB    | 40:J:83:THR:OG1   | 2.20                     | 0.40              |
| 41:K:127:ARG:HG2  | 41:K:127:ARG:NH1  | 2.36                     | 0.40              |
| 43:M:29:SER:O     | 43:M:32:ILE:HB    | 2.20                     | 0.40              |
| 45:O:47:LYS:C     | 45:O:49:HIS:H     | 2.30                     | 0.40              |
| 46:P:8:ARG:CZ     | 46:P:15:PRO:HB3   | 2.52                     | 0.40              |
| 46:P:14:ARG:HH21  | 46:P:42:ILE:HD12  | 1.85                     | 0.40              |
| 46:P:48:GLU:CG    | 46:P:49:GLY:N     | 2.83                     | 0.40              |
| 51:U:23:GLU:HG3   | 51:U:24:LYS:N     | 2.37                     | 0.40              |
| 51:U:38:GLU:C     | 51:U:40:PRO:CD    | 2.94                     | 0.40              |
| 52:03:63:THR:HG21 | 52:03:192:LEU:CD1 | 2.51                     | 0.40              |
| 53:A:129:A:H1'    | 53:A:130:A:C8     | 2.57                     | 0.40              |
| 53:A:502:A:H2'    | 53:A:503:C:O4'    | 2.21                     | 0.40              |
| 53:A:900:A:H2'    | 53:A:901:A:C8     | 2.57                     | 0.40              |
| 53:A:1326:U:H2'   | 53:A:1327:C:H6    | 1.86                     | 0.40              |
| 54:01:566:U:H2'   | 54:01:567:U:O4'   | 2.22                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 54:01:672:C:O2'   | 54:01:673:C:H5'  | 2.22                     | 0.40              |
| 54:01:819:A:C5    | 54:01:1189:A:C2  | 3.10                     | 0.40              |
| 54:01:1083:U:H2'  | 54:01:1085:A:OP2 | 2.20                     | 0.40              |
| 54:01:1161:C:H2'  | 54:01:1162:G:H8  | 1.86                     | 0.40              |
| 54:01:1339:G:H2'  | 54:01:1340:U:O2  | 2.22                     | 0.40              |
| 54:01:1433:A:O2'  | 54:01:1434:A:H5' | 2.21                     | 0.40              |
| 54:01:1680:U:C2'  | 54:01:1681:G:H5' | 2.52                     | 0.40              |
| 54:01:2547:A:H2'  | 54:01:2548:U:C6  | 2.56                     | 0.40              |
| 59:Z:131:LEU:HD12 | 59:Z:131:LEU:N   | 2.36                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | 04    | 269/271 (99%) | 225 (84%) | 33 (12%) | 11 (4%)  | 2           | 19 |
| 2   | 05    | 207/209 (99%) | 175 (84%) | 31 (15%) | 1 (0%)   | 24          | 57 |
| 3   | 06    | 199/201 (99%) | 164 (82%) | 29 (15%) | 6 (3%)   | 3           | 25 |
| 4   | 07    | 175/177 (99%) | 140 (80%) | 31 (18%) | 4 (2%)   | 5           | 30 |
| 5   | 08    | 174/176 (99%) | 155 (89%) | 17 (10%) | 2 (1%)   | 11          | 43 |
| 6   | 09    | 147/149 (99%) | 111 (76%) | 27 (18%) | 9 (6%)   | 1           | 12 |
| 7   | 10    | 129/131 (98%) | 98 (76%)  | 25 (19%) | 6 (5%)   | 2           | 17 |
| 8   | 11    | 139/141 (99%) | 118 (85%) | 18 (13%) | 3 (2%)   | 5           | 30 |
| 9   | 12    | 140/142 (99%) | 122 (87%) | 13 (9%)  | 5 (4%)   | 2           | 22 |
| 10  | 13    | 120/122 (98%) | 103 (86%) | 15 (12%) | 2 (2%)   | 7           | 35 |
| 11  | 14    | 141/143 (99%) | 120 (85%) | 19 (14%) | 2 (1%)   | 9           | 38 |
| 12  | 15    | 134/136 (98%) | 103 (77%) | 26 (19%) | 5 (4%)   | 2           | 21 |
| 13  | 16    | 118/120 (98%) | 83 (70%)  | 30 (25%) | 5 (4%)   | 2           | 19 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 14  | 17    | 114/116 (98%) | 95 (83%)  | 14 (12%) | 5 (4%)   | 2           | 17  |
| 15  | 18    | 112/114 (98%) | 89 (80%)  | 18 (16%) | 5 (4%)   | 2           | 17  |
| 16  | 19    | 115/117 (98%) | 94 (82%)  | 17 (15%) | 4 (4%)   | 3           | 23  |
| 17  | 20    | 101/103 (98%) | 86 (85%)  | 11 (11%) | 4 (4%)   | 2           | 19  |
| 18  | 21    | 108/110 (98%) | 87 (81%)  | 17 (16%) | 4 (4%)   | 2           | 21  |
| 19  | 22    | 91/93 (98%)   | 78 (86%)  | 13 (14%) | 0        | 100         | 100 |
| 20  | 23    | 100/102 (98%) | 81 (81%)  | 15 (15%) | 4 (4%)   | 2           | 19  |
| 21  | 24    | 92/94 (98%)   | 78 (85%)  | 11 (12%) | 3 (3%)   | 3           | 23  |
| 22  | 25    | 73/75 (97%)   | 65 (89%)  | 8 (11%)  | 0        | 100         | 100 |
| 23  | 26    | 75/77 (97%)   | 67 (89%)  | 7 (9%)   | 1 (1%)   | 9           | 39  |
| 24  | 27    | 61/63 (97%)   | 48 (79%)  | 10 (16%) | 3 (5%)   | 1           | 16  |
| 25  | 28    | 56/58 (97%)   | 49 (88%)  | 7 (12%)  | 0        | 100         | 100 |
| 26  | 29    | 64/66 (97%)   | 53 (83%)  | 9 (14%)  | 2 (3%)   | 3           | 25  |
| 27  | 30    | 54/56 (96%)   | 46 (85%)  | 6 (11%)  | 2 (4%)   | 2           | 21  |
| 28  | 31    | 48/50 (96%)   | 42 (88%)  | 6 (12%)  | 0        | 100         | 100 |
| 29  | 32    | 44/46 (96%)   | 29 (66%)  | 11 (25%) | 4 (9%)   | 0           | 7   |
| 30  | 33    | 62/64 (97%)   | 50 (81%)  | 7 (11%)  | 5 (8%)   | 1           | 8   |
| 31  | 34    | 36/38 (95%)   | 29 (81%)  | 7 (19%)  | 0        | 100         | 100 |
| 32  | B     | 223/225 (99%) | 193 (86%) | 26 (12%) | 4 (2%)   | 6           | 34  |
| 33  | C     | 204/206 (99%) | 167 (82%) | 29 (14%) | 8 (4%)   | 2           | 20  |
| 34  | D     | 203/205 (99%) | 157 (77%) | 32 (16%) | 14 (7%)  | 1           | 10  |
| 35  | E     | 155/157 (99%) | 123 (79%) | 24 (16%) | 8 (5%)   | 1           | 14  |
| 36  | F     | 124/126 (98%) | 101 (82%) | 17 (14%) | 6 (5%)   | 2           | 16  |
| 37  | G     | 149/151 (99%) | 125 (84%) | 21 (14%) | 3 (2%)   | 6           | 32  |
| 38  | H     | 127/129 (98%) | 109 (86%) | 16 (13%) | 2 (2%)   | 7           | 36  |
| 39  | I     | 125/127 (98%) | 101 (81%) | 16 (13%) | 8 (6%)   | 1           | 11  |
| 40  | J     | 96/98 (98%)   | 82 (85%)  | 11 (12%) | 3 (3%)   | 3           | 25  |
| 41  | K     | 114/116 (98%) | 92 (81%)  | 19 (17%) | 3 (3%)   | 4           | 27  |
| 42  | L     | 121/123 (98%) | 93 (77%)  | 20 (16%) | 8 (7%)   | 1           | 11  |
| 43  | M     | 112/114 (98%) | 88 (79%)  | 20 (18%) | 4 (4%)   | 2           | 22  |
| 44  | N     | 98/100 (98%)  | 70 (71%)  | 24 (24%) | 4 (4%)   | 2           | 19  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 45  | O     | 86/88 (98%)     | 64 (74%)   | 20 (23%)  | 2 (2%)   | 5           | 30 |
| 46  | P     | 80/82 (98%)     | 62 (78%)   | 17 (21%)  | 1 (1%)   | 9           | 39 |
| 47  | Q     | 78/80 (98%)     | 61 (78%)   | 14 (18%)  | 3 (4%)   | 2           | 20 |
| 48  | R     | 63/65 (97%)     | 50 (79%)   | 8 (13%)   | 5 (8%)   | 1           | 8  |
| 49  | S     | 77/79 (98%)     | 63 (82%)   | 9 (12%)   | 5 (6%)   | 1           | 11 |
| 50  | T     | 83/85 (98%)     | 74 (89%)   | 8 (10%)   | 1 (1%)   | 10          | 41 |
| 51  | U     | 63/65 (97%)     | 42 (67%)   | 19 (30%)  | 2 (3%)   | 3           | 24 |
| 52  | 03    | 130/223 (58%)   | 114 (88%)  | 13 (10%)  | 3 (2%)   | 5           | 30 |
| 59  | Z     | 150/554 (27%)   | 126 (84%)  | 21 (14%)  | 3 (2%)   | 6           | 32 |
| All | All   | 6159/6758 (91%) | 5040 (82%) | 912 (15%) | 207 (3%) | 4           | 23 |

All (207) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 04    | 261 | ARG  |
| 3   | 06    | 84  | THR  |
| 4   | 07    | 175 | PRO  |
| 6   | 09    | 10  | ALA  |
| 7   | 10    | 58  | THR  |
| 7   | 10    | 118 | ILE  |
| 11  | 14    | 85  | VAL  |
| 13  | 16    | 14  | SER  |
| 17  | 20    | 38  | VAL  |
| 17  | 20    | 54  | VAL  |
| 26  | 29    | 51  | VAL  |
| 29  | 32    | 5   | PHE  |
| 33  | C     | 60  | ALA  |
| 33  | C     | 112 | ALA  |
| 34  | D     | 169 | TRP  |
| 35  | E     | 25  | LYS  |
| 35  | E     | 122 | VAL  |
| 36  | F     | 54  | LEU  |
| 39  | I     | 71  | ILE  |
| 39  | I     | 90  | ASP  |
| 42  | L     | 75  | GLU  |
| 1   | 04    | 236 | GLY  |
| 1   | 04    | 240 | GLY  |
| 3   | 06    | 80  | SER  |
| 4   | 07    | 20  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 09    | 9   | VAL  |
| 6   | 09    | 91  | PHE  |
| 6   | 09    | 118 | PRO  |
| 7   | 10    | 108 | VAL  |
| 8   | 11    | 3   | LYS  |
| 8   | 11    | 12  | VAL  |
| 9   | 12    | 22  | GLY  |
| 9   | 12    | 81  | ILE  |
| 9   | 12    | 100 | VAL  |
| 10  | 13    | 106 | GLU  |
| 13  | 16    | 2   | ARG  |
| 14  | 17    | 15  | ARG  |
| 15  | 18    | 53  | GLY  |
| 15  | 18    | 93  | LYS  |
| 15  | 18    | 97  | TYR  |
| 17  | 20    | 69  | GLY  |
| 18  | 21    | 12  | SER  |
| 20  | 23    | 6   | ARG  |
| 24  | 27    | 2   | LYS  |
| 24  | 27    | 24  | GLU  |
| 24  | 27    | 25  | GLN  |
| 27  | 30    | 53  | VAL  |
| 30  | 33    | 7   | ARG  |
| 34  | D     | 26  | ALA  |
| 34  | D     | 68  | GLU  |
| 34  | D     | 191 | SER  |
| 35  | E     | 11  | GLN  |
| 35  | E     | 26  | GLY  |
| 35  | E     | 93  | VAL  |
| 36  | F     | 56  | LYS  |
| 37  | G     | 95  | ARG  |
| 39  | I     | 12  | LYS  |
| 39  | I     | 57  | VAL  |
| 39  | I     | 100 | ALA  |
| 39  | I     | 120 | ALA  |
| 41  | K     | 92  | ARG  |
| 42  | L     | 25  | ALA  |
| 42  | L     | 47  | ALA  |
| 42  | L     | 108 | ASP  |
| 44  | N     | 3   | GLN  |
| 45  | O     | 49  | HIS  |
| 47  | Q     | 70  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | R     | 13  | THR  |
| 48  | R     | 17  | VAL  |
| 49  | S     | 3   | SER  |
| 49  | S     | 7   | GLY  |
| 52  | 03    | 17  | ALA  |
| 52  | 03    | 189 | LEU  |
| 59  | Z     | 33  | LYS  |
| 1   | 04    | 147 | PRO  |
| 2   | 05    | 31  | ALA  |
| 3   | 06    | 83  | VAL  |
| 3   | 06    | 156 | ASN  |
| 3   | 06    | 182 | ALA  |
| 6   | 09    | 3   | VAL  |
| 6   | 09    | 38  | PRO  |
| 6   | 09    | 41  | LYS  |
| 6   | 09    | 136 | SER  |
| 7   | 10    | 107 | GLU  |
| 7   | 10    | 121 | SER  |
| 9   | 12    | 51  | GLY  |
| 12  | 15    | 45  | GLN  |
| 12  | 15    | 82  | MET  |
| 14  | 17    | 8   | ILE  |
| 14  | 17    | 69  | ASP  |
| 14  | 17    | 102 | ARG  |
| 15  | 18    | 18  | SER  |
| 18  | 21    | 65  | ASP  |
| 21  | 24    | 15  | GLY  |
| 23  | 26    | 31  | ASN  |
| 29  | 32    | 40  | ALA  |
| 30  | 33    | 62  | PRO  |
| 32  | B     | 19  | THR  |
| 32  | B     | 131 | LYS  |
| 33  | C     | 120 | THR  |
| 33  | C     | 156 | LEU  |
| 34  | D     | 22  | SER  |
| 34  | D     | 47  | LEU  |
| 34  | D     | 153 | ARG  |
| 34  | D     | 165 | GLU  |
| 35  | E     | 98  | ALA  |
| 36  | F     | 50  | PRO  |
| 38  | H     | 29  | SER  |
| 40  | J     | 89  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | L     | 23  | LEU  |
| 43  | M     | 15  | VAL  |
| 44  | N     | 43  | ALA  |
| 47  | Q     | 15  | LYS  |
| 48  | R     | 26  | ALA  |
| 48  | R     | 42  | ARG  |
| 49  | S     | 4   | LEU  |
| 1   | 04    | 31  | PRO  |
| 1   | 04    | 107 | LYS  |
| 1   | 04    | 116 | GLN  |
| 1   | 04    | 231 | HIS  |
| 1   | 04    | 260 | LYS  |
| 4   | 07    | 2   | LYS  |
| 5   | 08    | 70  | LEU  |
| 8   | 11    | 35  | MET  |
| 10  | 13    | 35  | VAL  |
| 11  | 14    | 29  | LYS  |
| 12  | 15    | 60  | GLN  |
| 13  | 16    | 46  | ARG  |
| 16  | 19    | 27  | ARG  |
| 16  | 19    | 78  | PHE  |
| 17  | 20    | 55  | ASP  |
| 18  | 21    | 90  | LYS  |
| 20  | 23    | 51  | LEU  |
| 30  | 33    | 29  | ARG  |
| 32  | B     | 165 | ALA  |
| 33  | C     | 28  | PHE  |
| 34  | D     | 20  | LEU  |
| 34  | D     | 36  | ALA  |
| 35  | E     | 112 | ALA  |
| 37  | G     | 4   | ARG  |
| 37  | G     | 58  | LEU  |
| 39  | I     | 91  | GLU  |
| 40  | J     | 16  | ARG  |
| 41  | K     | 88  | PRO  |
| 42  | L     | 90  | PRO  |
| 44  | N     | 19  | TYR  |
| 44  | N     | 34  | ASN  |
| 48  | R     | 20  | ILE  |
| 49  | S     | 70  | LEU  |
| 50  | T     | 3   | ILE  |
| 51  | U     | 34  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59  | Z     | 116 | VAL  |
| 1   | 04    | 164 | VAL  |
| 1   | 04    | 226 | PRO  |
| 5   | 08    | 174 | LYS  |
| 6   | 09    | 25  | TYR  |
| 12  | 15    | 69  | PRO  |
| 16  | 19    | 55  | GLN  |
| 20  | 23    | 99  | SER  |
| 27  | 30    | 17  | SER  |
| 29  | 32    | 25  | LYS  |
| 29  | 32    | 45  | SER  |
| 30  | 33    | 27  | ASN  |
| 34  | D     | 4   | LEU  |
| 35  | E     | 132 | PRO  |
| 36  | F     | 13  | ASP  |
| 36  | F     | 94  | HIS  |
| 36  | F     | 100 | SER  |
| 38  | H     | 96  | ALA  |
| 42  | L     | 35  | ARG  |
| 42  | L     | 43  | LYS  |
| 43  | M     | 69  | ARG  |
| 43  | M     | 113 | LYS  |
| 47  | Q     | 17  | GLU  |
| 51  | U     | 19  | LYS  |
| 52  | 03    | 23  | ILE  |
| 59  | Z     | 89  | ALA  |
| 3   | 06    | 35  | TYR  |
| 9   | 12    | 133 | ALA  |
| 13  | 16    | 60  | VAL  |
| 14  | 17    | 68  | LYS  |
| 16  | 19    | 76  | SER  |
| 26  | 29    | 28  | VAL  |
| 33  | C     | 13  | ILE  |
| 43  | M     | 7   | ASN  |
| 46  | P     | 13  | LYS  |
| 7   | 10    | 55  | VAL  |
| 15  | 18    | 17  | PRO  |
| 33  | C     | 8   | GLY  |
| 34  | D     | 167 | PRO  |
| 41  | K     | 91  | GLY  |
| 12  | 15    | 46  | ILE  |
| 13  | 16    | 109 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | 23    | 47  | PRO  |
| 21  | 24    | 84  | PRO  |
| 32  | B     | 148 | GLY  |
| 4   | 07    | 11  | VAL  |
| 18  | 21    | 55  | ILE  |
| 30  | 33    | 31  | ILE  |
| 33  | C     | 59  | PRO  |
| 34  | D     | 6   | PRO  |
| 21  | 24    | 81  | PRO  |
| 39  | I     | 54  | VAL  |
| 40  | J     | 57  | VAL  |
| 45  | O     | 26  | VAL  |
| 49  | S     | 75  | PRO  |
| 34  | D     | 33  | ILE  |

### 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   | 04    | 216/216 (100%) | 216 (100%) | 0        | 100         | 100 |
| 2   | 05    | 164/164 (100%) | 164 (100%) | 0        | 100         | 100 |
| 3   | 06    | 165/165 (100%) | 165 (100%) | 0        | 100         | 100 |
| 4   | 07    | 148/148 (100%) | 146 (99%)  | 2 (1%)   | 59          | 71  |
| 5   | 08    | 137/137 (100%) | 137 (100%) | 0        | 100         | 100 |
| 6   | 09    | 114/114 (100%) | 114 (100%) | 0        | 100         | 100 |
| 7   | 10    | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 8   | 11    | 109/109 (100%) | 108 (99%)  | 1 (1%)   | 70          | 76  |
| 9   | 12    | 116/116 (100%) | 114 (98%)  | 2 (2%)   | 53          | 70  |
| 10  | 13    | 103/103 (100%) | 103 (100%) | 0        | 100         | 100 |
| 11  | 14    | 102/102 (100%) | 99 (97%)   | 3 (3%)   | 37          | 60  |
| 12  | 15    | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 13  | 16    | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 14  | 17    | 86/86 (100%)   | 86 (100%)  | 0        | 100         | 100 |
| 15  | 18    | 99/99 (100%)   | 98 (99%)   | 1 (1%)   | 68          | 75  |
| 16  | 19    | 89/89 (100%)   | 89 (100%)  | 0        | 100         | 100 |
| 17  | 20    | 84/84 (100%)   | 83 (99%)   | 1 (1%)   | 63          | 73  |
| 18  | 21    | 93/93 (100%)   | 93 (100%)  | 0        | 100         | 100 |
| 19  | 22    | 80/80 (100%)   | 80 (100%)  | 0        | 100         | 100 |
| 20  | 23    | 83/83 (100%)   | 81 (98%)   | 2 (2%)   | 43          | 64  |
| 21  | 24    | 78/78 (100%)   | 77 (99%)   | 1 (1%)   | 61          | 72  |
| 22  | 25    | 57/57 (100%)   | 57 (100%)  | 0        | 100         | 100 |
| 23  | 26    | 67/67 (100%)   | 66 (98%)   | 1 (2%)   | 57          | 71  |
| 24  | 27    | 55/55 (100%)   | 55 (100%)  | 0        | 100         | 100 |
| 25  | 28    | 48/48 (100%)   | 48 (100%)  | 0        | 100         | 100 |
| 26  | 29    | 59/59 (100%)   | 59 (100%)  | 0        | 100         | 100 |
| 27  | 30    | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 28  | 31    | 45/45 (100%)   | 44 (98%)   | 1 (2%)   | 45          | 65  |
| 29  | 32    | 38/38 (100%)   | 38 (100%)  | 0        | 100         | 100 |
| 30  | 33    | 51/51 (100%)   | 51 (100%)  | 0        | 100         | 100 |
| 31  | 34    | 34/34 (100%)   | 34 (100%)  | 0        | 100         | 100 |
| 32  | B     | 186/186 (100%) | 185 (100%) | 1 (0%)   | 81          | 80  |
| 33  | C     | 170/170 (100%) | 170 (100%) | 0        | 100         | 100 |
| 34  | D     | 172/172 (100%) | 167 (97%)  | 5 (3%)   | 37          | 60  |
| 35  | E     | 119/119 (100%) | 117 (98%)  | 2 (2%)   | 53          | 70  |
| 36  | F     | 108/108 (100%) | 107 (99%)  | 1 (1%)   | 70          | 76  |
| 37  | G     | 124/124 (100%) | 124 (100%) | 0        | 100         | 100 |
| 38  | H     | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 39  | I     | 105/105 (100%) | 104 (99%)  | 1 (1%)   | 68          | 75  |
| 40  | J     | 86/86 (100%)   | 85 (99%)   | 1 (1%)   | 63          | 73  |
| 41  | K     | 89/89 (100%)   | 89 (100%)  | 0        | 100         | 100 |
| 42  | L     | 103/103 (100%) | 103 (100%) | 0        | 100         | 100 |
| 43  | M     | 92/92 (100%)   | 92 (100%)  | 0        | 100         | 100 |
| 44  | N     | 83/83 (100%)   | 82 (99%)   | 1 (1%)   | 63          | 73  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 45  | O     | 76/76 (100%)    | 76 (100%)  | 0        | 100         | 100 |
| 46  | P     | 65/65 (100%)    | 63 (97%)   | 2 (3%)   | 35          | 59  |
| 47  | Q     | 74/74 (100%)    | 74 (100%)  | 0        | 100         | 100 |
| 48  | R     | 56/56 (100%)    | 56 (100%)  | 0        | 100         | 100 |
| 49  | S     | 70/70 (100%)    | 70 (100%)  | 0        | 100         | 100 |
| 50  | T     | 65/65 (100%)    | 65 (100%)  | 0        | 100         | 100 |
| 51  | U     | 55/55 (100%)    | 55 (100%)  | 0        | 100         | 100 |
| 52  | 03    | 110/174 (63%)   | 109 (99%)  | 1 (1%)   | 70          | 76  |
| 59  | Z     | 129/458 (28%)   | 123 (95%)  | 6 (5%)   | 23          | 49  |
| All | All   | 5117/5510 (93%) | 5081 (99%) | 36 (1%)  | 73          | 78  |

All (36) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 07    | 140 | ILE  |
| 4   | 07    | 175 | PRO  |
| 8   | 11    | 128 | ILE  |
| 9   | 12    | 84  | ILE  |
| 9   | 12    | 101 | ILE  |
| 11  | 14    | 14  | LYS  |
| 11  | 14    | 23  | ILE  |
| 11  | 14    | 111 | ILE  |
| 15  | 18    | 3   | ILE  |
| 17  | 20    | 74  | ILE  |
| 20  | 23    | 4   | ILE  |
| 20  | 23    | 82  | VAL  |
| 21  | 24    | 81  | PRO  |
| 23  | 26    | 22  | ASN  |
| 28  | 31    | 4   | ILE  |
| 32  | B     | 202 | ASN  |
| 34  | D     | 27  | ILE  |
| 34  | D     | 28  | ASP  |
| 34  | D     | 87  | GLU  |
| 34  | D     | 131 | ILE  |
| 34  | D     | 144 | ILE  |
| 35  | E     | 15  | ILE  |
| 35  | E     | 133 | ILE  |
| 36  | F     | 111 | GLU  |
| 39  | I     | 60  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | J     | 75  | ASP  |
| 44  | N     | 92  | ILE  |
| 46  | P     | 29  | ASN  |
| 46  | P     | 33  | ILE  |
| 52  | 03    | 214 | ILE  |
| 59  | Z     | 100 | LYS  |
| 59  | Z     | 121 | THR  |
| 59  | Z     | 130 | PHE  |
| 59  | Z     | 148 | GLU  |
| 59  | Z     | 150 | LYS  |
| 59  | Z     | 162 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 04    | 20  | ASN  |
| 1   | 04    | 24  | HIS  |
| 1   | 04    | 44  | ASN  |
| 1   | 04    | 45  | ASN  |
| 1   | 04    | 52  | HIS  |
| 1   | 04    | 59  | GLN  |
| 1   | 04    | 85  | ASN  |
| 1   | 04    | 89  | ASN  |
| 1   | 04    | 116 | GLN  |
| 1   | 04    | 127 | ASN  |
| 1   | 04    | 133 | ASN  |
| 1   | 04    | 142 | ASN  |
| 1   | 04    | 152 | GLN  |
| 1   | 04    | 162 | GLN  |
| 1   | 04    | 196 | ASN  |
| 1   | 04    | 225 | ASN  |
| 1   | 04    | 238 | ASN  |
| 2   | 05    | 32  | ASN  |
| 2   | 05    | 42  | ASN  |
| 2   | 05    | 148 | GLN  |
| 3   | 06    | 24  | ASN  |
| 3   | 06    | 46  | GLN  |
| 3   | 06    | 62  | GLN  |
| 3   | 06    | 90  | GLN  |
| 3   | 06    | 97  | ASN  |
| 3   | 06    | 156 | ASN  |
| 4   | 07    | 20  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 07    | 26  | GLN  |
| 4   | 07    | 51  | ASN  |
| 5   | 08    | 21  | GLN  |
| 5   | 08    | 37  | ASN  |
| 5   | 08    | 63  | GLN  |
| 5   | 08    | 103 | ASN  |
| 5   | 08    | 138 | GLN  |
| 6   | 09    | 2   | GLN  |
| 6   | 09    | 18  | GLN  |
| 6   | 09    | 28  | ASN  |
| 6   | 09    | 66  | ASN  |
| 6   | 09    | 73  | ASN  |
| 6   | 09    | 135 | HIS  |
| 7   | 10    | 4   | ASN  |
| 7   | 10    | 57  | ASN  |
| 8   | 11    | 93  | ASN  |
| 9   | 12    | 58  | ASN  |
| 10  | 13    | 13  | ASN  |
| 10  | 13    | 88  | ASN  |
| 11  | 14    | 38  | GLN  |
| 11  | 14    | 54  | GLN  |
| 11  | 14    | 99  | ASN  |
| 12  | 15    | 3   | GLN  |
| 12  | 15    | 60  | GLN  |
| 13  | 16    | 9   | GLN  |
| 13  | 16    | 31  | HIS  |
| 13  | 16    | 81  | ASN  |
| 13  | 16    | 107 | ASN  |
| 14  | 17    | 29  | HIS  |
| 15  | 18    | 6   | GLN  |
| 15  | 18    | 11  | GLN  |
| 15  | 18    | 51  | ASN  |
| 16  | 19    | 19  | GLN  |
| 16  | 19    | 51  | GLN  |
| 16  | 19    | 55  | GLN  |
| 16  | 19    | 80  | ASN  |
| 17  | 20    | 18  | GLN  |
| 17  | 20    | 87  | GLN  |
| 17  | 20    | 89  | HIS  |
| 18  | 21    | 40  | ASN  |
| 19  | 22    | 59  | ASN  |
| 20  | 23    | 65  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | 23    | 68  | ASN  |
| 20  | 23    | 73  | ASN  |
| 20  | 23    | 98  | ASN  |
| 21  | 24    | 24  | ASN  |
| 21  | 24    | 87  | GLN  |
| 23  | 26    | 22  | ASN  |
| 23  | 26    | 31  | ASN  |
| 24  | 27    | 27  | ASN  |
| 24  | 27    | 41  | HIS  |
| 25  | 28    | 8   | GLN  |
| 26  | 29    | 61  | ASN  |
| 27  | 30    | 3   | GLN  |
| 27  | 30    | 4   | GLN  |
| 27  | 30    | 18  | HIS  |
| 29  | 32    | 16  | HIS  |
| 32  | B     | 18  | GLN  |
| 32  | B     | 38  | HIS  |
| 32  | B     | 50  | ASN  |
| 32  | B     | 57  | ASN  |
| 32  | B     | 145 | ASN  |
| 32  | B     | 167 | HIS  |
| 32  | B     | 176 | ASN  |
| 32  | B     | 202 | ASN  |
| 33  | C     | 24  | ASN  |
| 33  | C     | 31  | ASN  |
| 33  | C     | 99  | GLN  |
| 33  | C     | 122 | GLN  |
| 33  | C     | 139 | ASN  |
| 33  | C     | 184 | ASN  |
| 34  | D     | 39  | GLN  |
| 34  | D     | 73  | ASN  |
| 34  | D     | 88  | ASN  |
| 34  | D     | 125 | ASN  |
| 34  | D     | 130 | ASN  |
| 34  | D     | 163 | GLN  |
| 34  | D     | 195 | ASN  |
| 34  | D     | 197 | HIS  |
| 35  | E     | 81  | GLN  |
| 36  | F     | 3   | HIS  |
| 36  | F     | 37  | HIS  |
| 36  | F     | 55  | HIS  |
| 36  | F     | 118 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | G     | 121 | ASN  |
| 38  | H     | 17  | GLN  |
| 38  | H     | 20  | ASN  |
| 39  | I     | 24  | ASN  |
| 39  | I     | 30  | ASN  |
| 39  | I     | 49  | GLN  |
| 39  | I     | 80  | HIS  |
| 40  | J     | 58  | ASN  |
| 40  | J     | 70  | HIS  |
| 41  | K     | 23  | HIS  |
| 41  | K     | 39  | ASN  |
| 41  | K     | 118 | ASN  |
| 42  | L     | 45  | ASN  |
| 42  | L     | 95  | HIS  |
| 43  | M     | 7   | ASN  |
| 43  | M     | 11  | HIS  |
| 43  | M     | 99  | GLN  |
| 44  | N     | 42  | ASN  |
| 44  | N     | 48  | GLN  |
| 45  | O     | 49  | HIS  |
| 46  | P     | 18  | GLN  |
| 46  | P     | 26  | ASN  |
| 46  | P     | 29  | ASN  |
| 47  | Q     | 8   | GLN  |
| 47  | Q     | 30  | HIS  |
| 48  | R     | 18  | GLN  |
| 48  | R     | 30  | ASN  |
| 48  | R     | 73  | HIS  |
| 49  | S     | 56  | HIS  |
| 49  | S     | 68  | HIS  |
| 50  | T     | 20  | ASN  |
| 50  | T     | 51  | ASN  |
| 50  | T     | 60  | GLN  |
| 50  | T     | 69  | ASN  |
| 50  | T     | 83  | ASN  |
| 52  | 03    | 24  | ASN  |
| 52  | 03    | 57  | GLN  |
| 52  | 03    | 58  | ASN  |
| 52  | 03    | 168 | ASN  |
| 59  | Z     | 178 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 53  | A     | 1538/1539 (99%) | 135 (8%)          | 4 (0%)          |
| 54  | 01    | 2902/2903 (99%) | 345 (11%)         | 10 (0%)         |
| 55  | 02    | 119/120 (99%)   | 12 (10%)          | 1 (0%)          |
| 56  | W     | 76/77 (98%)     | 7 (9%)            | 0               |
| 56  | X     | 76/77 (98%)     | 15 (19%)          | 0               |
| 57  | V     | 17/27 (62%)     | 3 (17%)           | 0               |
| 58  | Y     | 75/76 (98%)     | 14 (18%)          | 1 (1%)          |
| All | All   | 4803/4819 (99%) | 531 (11%)         | 16 (0%)         |

All (531) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | A     | 6   | G    |
| 53  | A     | 9   | G    |
| 53  | A     | 22  | G    |
| 53  | A     | 31  | G    |
| 53  | A     | 32  | A    |
| 53  | A     | 39  | G    |
| 53  | A     | 48  | C    |
| 53  | A     | 51  | A    |
| 53  | A     | 71  | A    |
| 53  | A     | 87  | C    |
| 53  | A     | 130 | A    |
| 53  | A     | 144 | G    |
| 53  | A     | 183 | C    |
| 53  | A     | 184 | G    |
| 53  | A     | 197 | A    |
| 53  | A     | 209 | U    |
| 53  | A     | 210 | C    |
| 53  | A     | 226 | G    |
| 53  | A     | 247 | G    |
| 53  | A     | 251 | G    |
| 53  | A     | 266 | G    |
| 53  | A     | 267 | C    |
| 53  | A     | 281 | G    |
| 53  | A     | 289 | G    |
| 53  | A     | 345 | C    |
| 53  | A     | 352 | C    |
| 53  | A     | 367 | U    |
| 53  | A     | 372 | C    |
| 53  | A     | 412 | A    |
| 53  | A     | 413 | G    |
| 53  | A     | 429 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | A     | 467 | U    |
| 53  | A     | 479 | U    |
| 53  | A     | 484 | G    |
| 53  | A     | 485 | U    |
| 53  | A     | 486 | U    |
| 53  | A     | 497 | G    |
| 53  | A     | 518 | C    |
| 53  | A     | 532 | A    |
| 53  | A     | 547 | A    |
| 53  | A     | 561 | U    |
| 53  | A     | 572 | A    |
| 53  | A     | 573 | A    |
| 53  | A     | 575 | G    |
| 53  | A     | 576 | C    |
| 53  | A     | 577 | G    |
| 53  | A     | 633 | G    |
| 53  | A     | 665 | A    |
| 53  | A     | 688 | G    |
| 53  | A     | 702 | A    |
| 53  | A     | 703 | G    |
| 53  | A     | 724 | G    |
| 53  | A     | 755 | G    |
| 53  | A     | 777 | A    |
| 53  | A     | 805 | C    |
| 53  | A     | 815 | A    |
| 53  | A     | 817 | C    |
| 53  | A     | 818 | G    |
| 53  | A     | 819 | A    |
| 53  | A     | 821 | G    |
| 53  | A     | 843 | U    |
| 53  | A     | 844 | G    |
| 53  | A     | 846 | G    |
| 53  | A     | 871 | U    |
| 53  | A     | 873 | A    |
| 53  | A     | 890 | G    |
| 53  | A     | 902 | G    |
| 53  | A     | 926 | G    |
| 53  | A     | 934 | C    |
| 53  | A     | 935 | A    |
| 53  | A     | 960 | U    |
| 53  | A     | 961 | U    |
| 53  | A     | 966 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | A     | 969  | A    |
| 53  | A     | 971  | G    |
| 53  | A     | 975  | A    |
| 53  | A     | 976  | G    |
| 53  | A     | 977  | A    |
| 53  | A     | 992  | U    |
| 53  | A     | 993  | G    |
| 53  | A     | 1004 | A    |
| 53  | A     | 1028 | C    |
| 53  | A     | 1031 | C    |
| 53  | A     | 1033 | G    |
| 53  | A     | 1034 | G    |
| 53  | A     | 1053 | G    |
| 53  | A     | 1094 | G    |
| 53  | A     | 1101 | A    |
| 53  | A     | 1136 | C    |
| 53  | A     | 1137 | C    |
| 53  | A     | 1138 | G    |
| 53  | A     | 1139 | G    |
| 53  | A     | 1159 | U    |
| 53  | A     | 1168 | U    |
| 53  | A     | 1182 | G    |
| 53  | A     | 1184 | G    |
| 53  | A     | 1191 | A    |
| 53  | A     | 1196 | A    |
| 53  | A     | 1198 | G    |
| 53  | A     | 1201 | A    |
| 53  | A     | 1202 | U    |
| 53  | A     | 1225 | A    |
| 53  | A     | 1238 | A    |
| 53  | A     | 1240 | U    |
| 53  | A     | 1241 | G    |
| 53  | A     | 1253 | G    |
| 53  | A     | 1257 | A    |
| 53  | A     | 1258 | G    |
| 53  | A     | 1260 | G    |
| 53  | A     | 1275 | A    |
| 53  | A     | 1278 | G    |
| 53  | A     | 1280 | A    |
| 53  | A     | 1282 | C    |
| 53  | A     | 1286 | U    |
| 53  | A     | 1287 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | A     | 1300 | G    |
| 53  | A     | 1317 | C    |
| 53  | A     | 1346 | A    |
| 53  | A     | 1347 | G    |
| 53  | A     | 1363 | A    |
| 53  | A     | 1381 | U    |
| 53  | A     | 1395 | C    |
| 53  | A     | 1419 | G    |
| 53  | A     | 1446 | A    |
| 53  | A     | 1448 | C    |
| 53  | A     | 1452 | C    |
| 53  | A     | 1492 | A    |
| 53  | A     | 1502 | A    |
| 53  | A     | 1503 | A    |
| 53  | A     | 1506 | U    |
| 53  | A     | 1517 | G    |
| 53  | A     | 1529 | G    |
| 53  | A     | 1530 | G    |
| 53  | A     | 1533 | C    |
| 53  | A     | 1540 | U    |
| 54  | 01    | 10   | A    |
| 54  | 01    | 12   | U    |
| 54  | 01    | 34   | U    |
| 54  | 01    | 35   | G    |
| 54  | 01    | 49   | A    |
| 54  | 01    | 51   | G    |
| 54  | 01    | 63   | A    |
| 54  | 01    | 71   | A    |
| 54  | 01    | 74   | A    |
| 54  | 01    | 75   | G    |
| 54  | 01    | 119  | A    |
| 54  | 01    | 120  | U    |
| 54  | 01    | 140  | C    |
| 54  | 01    | 141  | G    |
| 54  | 01    | 142  | A    |
| 54  | 01    | 162  | U    |
| 54  | 01    | 163  | C    |
| 54  | 01    | 181  | A    |
| 54  | 01    | 196  | A    |
| 54  | 01    | 216  | A    |
| 54  | 01    | 221  | A    |
| 54  | 01    | 222  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | 01    | 228 | C    |
| 54  | 01    | 229 | C    |
| 54  | 01    | 248 | G    |
| 54  | 01    | 249 | C    |
| 54  | 01    | 255 | A    |
| 54  | 01    | 265 | A    |
| 54  | 01    | 266 | G    |
| 54  | 01    | 276 | U    |
| 54  | 01    | 278 | A    |
| 54  | 01    | 281 | C    |
| 54  | 01    | 294 | A    |
| 54  | 01    | 301 | G    |
| 54  | 01    | 311 | A    |
| 54  | 01    | 312 | G    |
| 54  | 01    | 323 | C    |
| 54  | 01    | 324 | A    |
| 54  | 01    | 329 | G    |
| 54  | 01    | 330 | A    |
| 54  | 01    | 361 | G    |
| 54  | 01    | 362 | A    |
| 54  | 01    | 371 | A    |
| 54  | 01    | 372 | G    |
| 54  | 01    | 386 | G    |
| 54  | 01    | 387 | U    |
| 54  | 01    | 404 | A    |
| 54  | 01    | 405 | U    |
| 54  | 01    | 406 | G    |
| 54  | 01    | 411 | G    |
| 54  | 01    | 412 | A    |
| 54  | 01    | 424 | G    |
| 54  | 01    | 451 | U    |
| 54  | 01    | 455 | C    |
| 54  | 01    | 458 | G    |
| 54  | 01    | 473 | G    |
| 54  | 01    | 480 | A    |
| 54  | 01    | 481 | G    |
| 54  | 01    | 491 | G    |
| 54  | 01    | 504 | A    |
| 54  | 01    | 505 | A    |
| 54  | 01    | 529 | A    |
| 54  | 01    | 531 | C    |
| 54  | 01    | 532 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | 01    | 543 | G    |
| 54  | 01    | 545 | U    |
| 54  | 01    | 563 | A    |
| 54  | 01    | 573 | U    |
| 54  | 01    | 588 | U    |
| 54  | 01    | 603 | A    |
| 54  | 01    | 614 | A    |
| 54  | 01    | 616 | A    |
| 54  | 01    | 627 | A    |
| 54  | 01    | 637 | A    |
| 54  | 01    | 646 | U    |
| 54  | 01    | 654 | A    |
| 54  | 01    | 669 | G    |
| 54  | 01    | 686 | U    |
| 54  | 01    | 687 | C    |
| 54  | 01    | 695 | G    |
| 54  | 01    | 730 | A    |
| 54  | 01    | 747 | C    |
| 54  | 01    | 752 | A    |
| 54  | 01    | 764 | A    |
| 54  | 01    | 776 | G    |
| 54  | 01    | 782 | A    |
| 54  | 01    | 784 | G    |
| 54  | 01    | 785 | G    |
| 54  | 01    | 805 | G    |
| 54  | 01    | 812 | C    |
| 54  | 01    | 819 | A    |
| 54  | 01    | 822 | G    |
| 54  | 01    | 827 | U    |
| 54  | 01    | 828 | U    |
| 54  | 01    | 830 | G    |
| 54  | 01    | 845 | A    |
| 54  | 01    | 846 | U    |
| 54  | 01    | 847 | U    |
| 54  | 01    | 859 | G    |
| 54  | 01    | 860 | U    |
| 54  | 01    | 878 | A    |
| 54  | 01    | 886 | A    |
| 54  | 01    | 887 | U    |
| 54  | 01    | 888 | C    |
| 54  | 01    | 896 | A    |
| 54  | 01    | 897 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | 01    | 910  | A    |
| 54  | 01    | 915  | C    |
| 54  | 01    | 932  | U    |
| 54  | 01    | 941  | A    |
| 54  | 01    | 945  | A    |
| 54  | 01    | 946  | C    |
| 54  | 01    | 961  | C    |
| 54  | 01    | 974  | G    |
| 54  | 01    | 975  | A    |
| 54  | 01    | 983  | A    |
| 54  | 01    | 995  | C    |
| 54  | 01    | 996  | A    |
| 54  | 01    | 1012 | U    |
| 54  | 01    | 1013 | C    |
| 54  | 01    | 1021 | A    |
| 54  | 01    | 1022 | G    |
| 54  | 01    | 1026 | G    |
| 54  | 01    | 1033 | U    |
| 54  | 01    | 1046 | A    |
| 54  | 01    | 1047 | G    |
| 54  | 01    | 1054 | A    |
| 54  | 01    | 1059 | G    |
| 54  | 01    | 1062 | G    |
| 54  | 01    | 1064 | C    |
| 54  | 01    | 1065 | U    |
| 54  | 01    | 1066 | U    |
| 54  | 01    | 1070 | A    |
| 54  | 01    | 1071 | G    |
| 54  | 01    | 1075 | C    |
| 54  | 01    | 1076 | C    |
| 54  | 01    | 1078 | U    |
| 54  | 01    | 1079 | C    |
| 54  | 01    | 1083 | U    |
| 54  | 01    | 1084 | A    |
| 54  | 01    | 1088 | A    |
| 54  | 01    | 1104 | C    |
| 54  | 01    | 1106 | G    |
| 54  | 01    | 1111 | A    |
| 54  | 01    | 1131 | G    |
| 54  | 01    | 1132 | U    |
| 54  | 01    | 1133 | A    |
| 54  | 01    | 1135 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | 01    | 1143 | A    |
| 54  | 01    | 1157 | G    |
| 54  | 01    | 1174 | U    |
| 54  | 01    | 1175 | A    |
| 54  | 01    | 1177 | G    |
| 54  | 01    | 1179 | G    |
| 54  | 01    | 1180 | U    |
| 54  | 01    | 1212 | G    |
| 54  | 01    | 1238 | G    |
| 54  | 01    | 1251 | C    |
| 54  | 01    | 1253 | A    |
| 54  | 01    | 1256 | G    |
| 54  | 01    | 1271 | G    |
| 54  | 01    | 1272 | A    |
| 54  | 01    | 1275 | A    |
| 54  | 01    | 1289 | C    |
| 54  | 01    | 1300 | G    |
| 54  | 01    | 1301 | A    |
| 54  | 01    | 1302 | A    |
| 54  | 01    | 1329 | U    |
| 54  | 01    | 1330 | C    |
| 54  | 01    | 1332 | G    |
| 54  | 01    | 1345 | C    |
| 54  | 01    | 1365 | A    |
| 54  | 01    | 1378 | A    |
| 54  | 01    | 1379 | U    |
| 54  | 01    | 1383 | A    |
| 54  | 01    | 1395 | A    |
| 54  | 01    | 1416 | G    |
| 54  | 01    | 1419 | A    |
| 54  | 01    | 1420 | A    |
| 54  | 01    | 1461 | C    |
| 54  | 01    | 1476 | U    |
| 54  | 01    | 1482 | G    |
| 54  | 01    | 1490 | A    |
| 54  | 01    | 1491 | G    |
| 54  | 01    | 1498 | C    |
| 54  | 01    | 1515 | A    |
| 54  | 01    | 1524 | G    |
| 54  | 01    | 1533 | C    |
| 54  | 01    | 1535 | A    |
| 54  | 01    | 1536 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | 01    | 1537 | G    |
| 54  | 01    | 1555 | G    |
| 54  | 01    | 1559 | U    |
| 54  | 01    | 1560 | G    |
| 54  | 01    | 1569 | A    |
| 54  | 01    | 1581 | G    |
| 54  | 01    | 1584 | U    |
| 54  | 01    | 1585 | C    |
| 54  | 01    | 1608 | A    |
| 54  | 01    | 1611 | C    |
| 54  | 01    | 1616 | A    |
| 54  | 01    | 1647 | U    |
| 54  | 01    | 1648 | U    |
| 54  | 01    | 1674 | G    |
| 54  | 01    | 1699 | G    |
| 54  | 01    | 1715 | G    |
| 54  | 01    | 1729 | U    |
| 54  | 01    | 1730 | C    |
| 54  | 01    | 1738 | G    |
| 54  | 01    | 1758 | U    |
| 54  | 01    | 1764 | C    |
| 54  | 01    | 1773 | A    |
| 54  | 01    | 1780 | A    |
| 54  | 01    | 1791 | A    |
| 54  | 01    | 1800 | C    |
| 54  | 01    | 1801 | A    |
| 54  | 01    | 1808 | A    |
| 54  | 01    | 1816 | C    |
| 54  | 01    | 1833 | C    |
| 54  | 01    | 1871 | A    |
| 54  | 01    | 1901 | A    |
| 54  | 01    | 1906 | G    |
| 54  | 01    | 1907 | G    |
| 54  | 01    | 1913 | A    |
| 54  | 01    | 1914 | C    |
| 54  | 01    | 1929 | G    |
| 54  | 01    | 1930 | G    |
| 54  | 01    | 1937 | A    |
| 54  | 01    | 1938 | A    |
| 54  | 01    | 1944 | U    |
| 54  | 01    | 1955 | U    |
| 54  | 01    | 1963 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | 01    | 1967 | C    |
| 54  | 01    | 1970 | A    |
| 54  | 01    | 1972 | G    |
| 54  | 01    | 1992 | G    |
| 54  | 01    | 1993 | U    |
| 54  | 01    | 1997 | C    |
| 54  | 01    | 2022 | U    |
| 54  | 01    | 2023 | C    |
| 54  | 01    | 2030 | A    |
| 54  | 01    | 2031 | A    |
| 54  | 01    | 2034 | U    |
| 54  | 01    | 2036 | C    |
| 54  | 01    | 2043 | C    |
| 54  | 01    | 2052 | A    |
| 54  | 01    | 2055 | C    |
| 54  | 01    | 2056 | G    |
| 54  | 01    | 2060 | A    |
| 54  | 01    | 2061 | G    |
| 54  | 01    | 2062 | A    |
| 54  | 01    | 2069 | G    |
| 54  | 01    | 2072 | C    |
| 54  | 01    | 2096 | C    |
| 54  | 01    | 2110 | G    |
| 54  | 01    | 2111 | U    |
| 54  | 01    | 2112 | G    |
| 54  | 01    | 2113 | U    |
| 54  | 01    | 2118 | U    |
| 54  | 01    | 2119 | A    |
| 54  | 01    | 2126 | A    |
| 54  | 01    | 2127 | G    |
| 54  | 01    | 2132 | U    |
| 54  | 01    | 2133 | G    |
| 54  | 01    | 2145 | C    |
| 54  | 01    | 2162 | G    |
| 54  | 01    | 2171 | A    |
| 54  | 01    | 2172 | U    |
| 54  | 01    | 2173 | A    |
| 54  | 01    | 2198 | A    |
| 54  | 01    | 2203 | U    |
| 54  | 01    | 2204 | G    |
| 54  | 01    | 2213 | U    |
| 54  | 01    | 2225 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | 01    | 2278 | A    |
| 54  | 01    | 2283 | C    |
| 54  | 01    | 2287 | A    |
| 54  | 01    | 2297 | A    |
| 54  | 01    | 2305 | U    |
| 54  | 01    | 2309 | A    |
| 54  | 01    | 2325 | G    |
| 54  | 01    | 2327 | A    |
| 54  | 01    | 2334 | U    |
| 54  | 01    | 2350 | C    |
| 54  | 01    | 2383 | G    |
| 54  | 01    | 2385 | C    |
| 54  | 01    | 2392 | A    |
| 54  | 01    | 2402 | U    |
| 54  | 01    | 2406 | A    |
| 54  | 01    | 2407 | A    |
| 54  | 01    | 2423 | U    |
| 54  | 01    | 2424 | C    |
| 54  | 01    | 2427 | C    |
| 54  | 01    | 2429 | G    |
| 54  | 01    | 2430 | A    |
| 54  | 01    | 2434 | A    |
| 54  | 01    | 2435 | A    |
| 54  | 01    | 2441 | U    |
| 54  | 01    | 2448 | A    |
| 54  | 01    | 2476 | A    |
| 54  | 01    | 2498 | C    |
| 54  | 01    | 2502 | G    |
| 54  | 01    | 2503 | A    |
| 54  | 01    | 2504 | U    |
| 54  | 01    | 2505 | G    |
| 54  | 01    | 2518 | A    |
| 54  | 01    | 2520 | C    |
| 54  | 01    | 2547 | A    |
| 54  | 01    | 2554 | U    |
| 54  | 01    | 2566 | A    |
| 54  | 01    | 2567 | G    |
| 54  | 01    | 2572 | A    |
| 54  | 01    | 2602 | A    |
| 54  | 01    | 2609 | U    |
| 54  | 01    | 2613 | U    |
| 54  | 01    | 2629 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 54  | 01    | 2646 | C    |
| 54  | 01    | 2655 | G    |
| 54  | 01    | 2682 | A    |
| 54  | 01    | 2689 | U    |
| 54  | 01    | 2690 | U    |
| 54  | 01    | 2714 | G    |
| 54  | 01    | 2716 | C    |
| 54  | 01    | 2744 | G    |
| 54  | 01    | 2748 | A    |
| 54  | 01    | 2764 | A    |
| 54  | 01    | 2765 | A    |
| 54  | 01    | 2778 | A    |
| 54  | 01    | 2779 | U    |
| 54  | 01    | 2791 | G    |
| 54  | 01    | 2797 | U    |
| 54  | 01    | 2799 | A    |
| 54  | 01    | 2800 | A    |
| 54  | 01    | 2809 | A    |
| 54  | 01    | 2820 | A    |
| 54  | 01    | 2821 | A    |
| 54  | 01    | 2833 | U    |
| 54  | 01    | 2849 | U    |
| 54  | 01    | 2850 | A    |
| 54  | 01    | 2867 | G    |
| 54  | 01    | 2868 | A    |
| 54  | 01    | 2872 | A    |
| 54  | 01    | 2879 | A    |
| 54  | 01    | 2880 | C    |
| 54  | 01    | 2883 | A    |
| 55  | 02    | 4    | C    |
| 55  | 02    | 13   | G    |
| 55  | 02    | 24   | G    |
| 55  | 02    | 35   | C    |
| 55  | 02    | 40   | U    |
| 55  | 02    | 41   | G    |
| 55  | 02    | 44   | G    |
| 55  | 02    | 67   | G    |
| 55  | 02    | 89   | U    |
| 55  | 02    | 90   | C    |
| 55  | 02    | 108  | A    |
| 55  | 02    | 109  | A    |
| 56  | X     | 2    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | X     | 3   | C    |
| 56  | X     | 8   | U    |
| 56  | X     | 9   | G    |
| 56  | X     | 10  | G    |
| 56  | X     | 14  | A    |
| 56  | X     | 19  | G    |
| 56  | X     | 20  | U    |
| 56  | X     | 21  | A    |
| 56  | X     | 22  | G    |
| 56  | X     | 34  | C    |
| 56  | X     | 46  | G    |
| 56  | X     | 61  | C    |
| 56  | X     | 64  | G    |
| 56  | X     | 70  | G    |
| 57  | V     | 12  | A    |
| 57  | V     | 13  | A    |
| 57  | V     | 16  | A    |
| 56  | W     | 9   | G    |
| 56  | W     | 19  | G    |
| 56  | W     | 20  | U    |
| 56  | W     | 47  | U    |
| 56  | W     | 48  | C    |
| 56  | W     | 61  | C    |
| 56  | W     | 76  | A    |
| 58  | Y     | 9   | A    |
| 58  | Y     | 17  | C    |
| 58  | Y     | 19  | G    |
| 58  | Y     | 21  | A    |
| 58  | Y     | 45  | U    |
| 58  | Y     | 46  | G    |
| 58  | Y     | 47  | U    |
| 58  | Y     | 48  | C    |
| 58  | Y     | 49  | C    |
| 58  | Y     | 59  | U    |
| 58  | Y     | 61  | C    |
| 58  | Y     | 64  | A    |
| 58  | Y     | 65  | G    |
| 58  | Y     | 74  | C    |

All (16) RNA pucker outliers are listed below:

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
|-----|-------|-----|------|

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | A     | 70   | U    |
| 53  | A     | 428  | G    |
| 53  | A     | 1190 | G    |
| 53  | A     | 1201 | A    |
| 54  | 01    | 227  | A    |
| 54  | 01    | 490  | C    |
| 54  | 01    | 859  | G    |
| 54  | 01    | 1020 | A    |
| 54  | 01    | 1130 | U    |
| 54  | 01    | 1475 | G    |
| 54  | 01    | 2286 | G    |
| 54  | 01    | 2296 | U    |
| 54  | 01    | 2326 | C    |
| 54  | 01    | 2391 | G    |
| 55  | 02    | 88   | C    |
| 58  | Y     | 63   | G    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 60  | FME  | W     | 101 | 56   | 8,9,10       | 0.67 | 0           | 8,9,11      | 1.01 | 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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 60  | FME  | W     | 101 | 56   | -       | 1/7/9/11 | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms     |
|-----|-------|-----|------|-----------|
| 60  | W     | 101 | FME  | O-C-CA-CB |

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

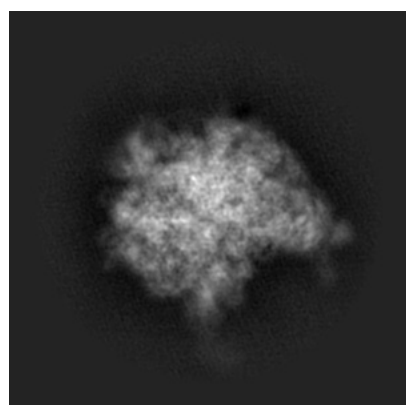
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7289. These allow visual inspection of the internal detail of the map and identification of artifacts.

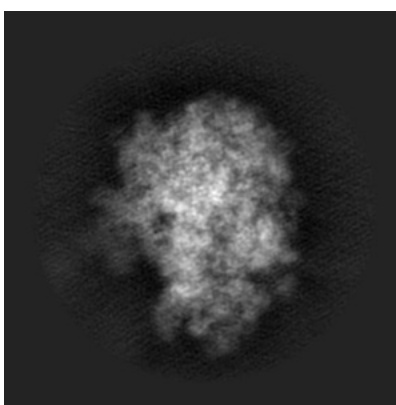
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

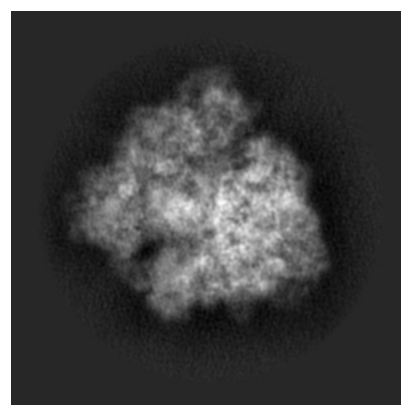
#### 6.1.1 Primary map



X



Y

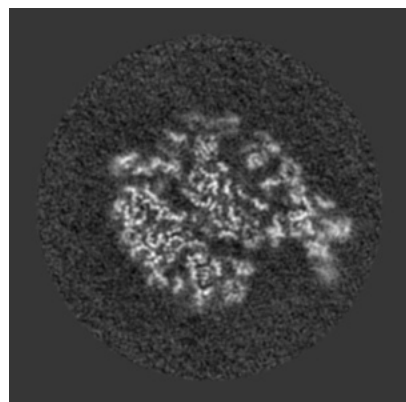


Z

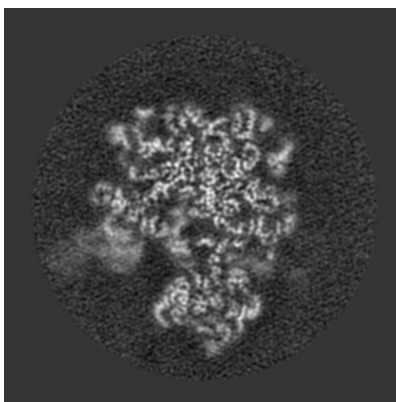
The images above show the map projected in three orthogonal directions.

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

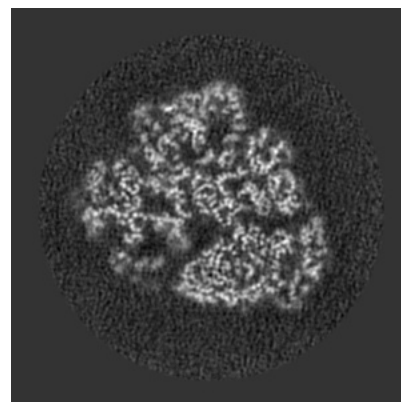
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

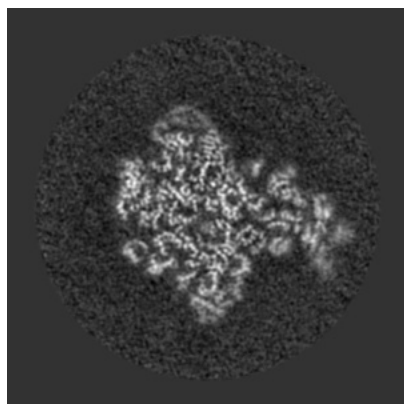


Z Index: 240

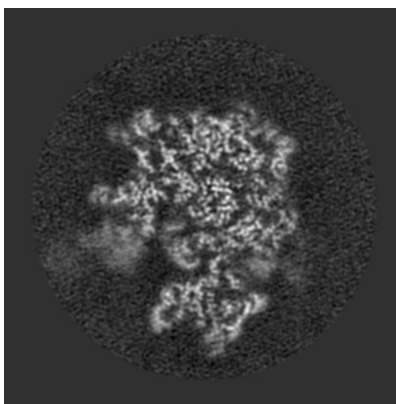
The images above show central slices of the map in three orthogonal directions.

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

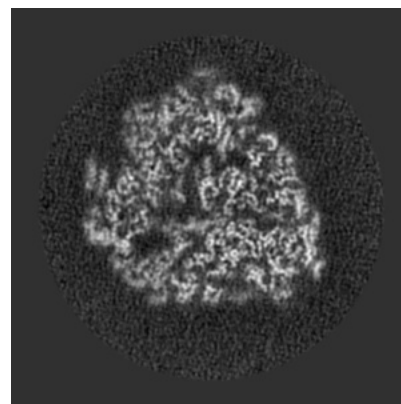
### 6.3.1 Primary map



X Index: 252



Y Index: 247

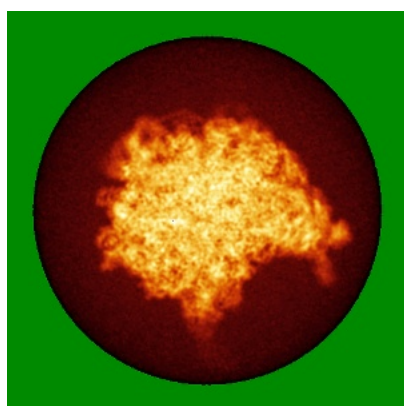


Z Index: 228

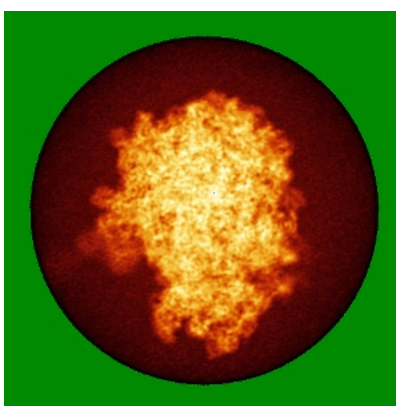
The images above show the largest variance slices of the map in three orthogonal directions.

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

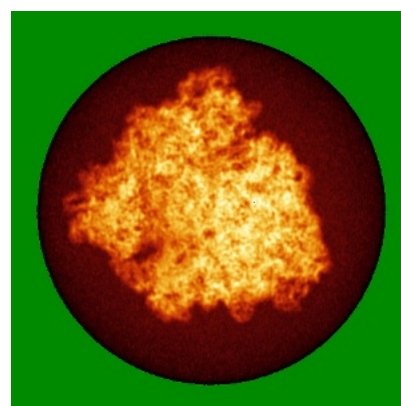
### 6.4.1 Primary map



X



Y

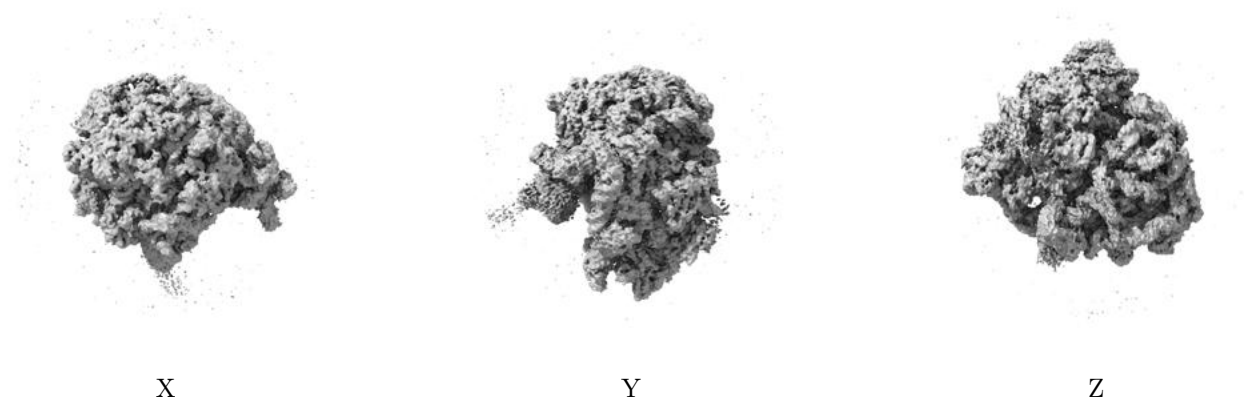


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

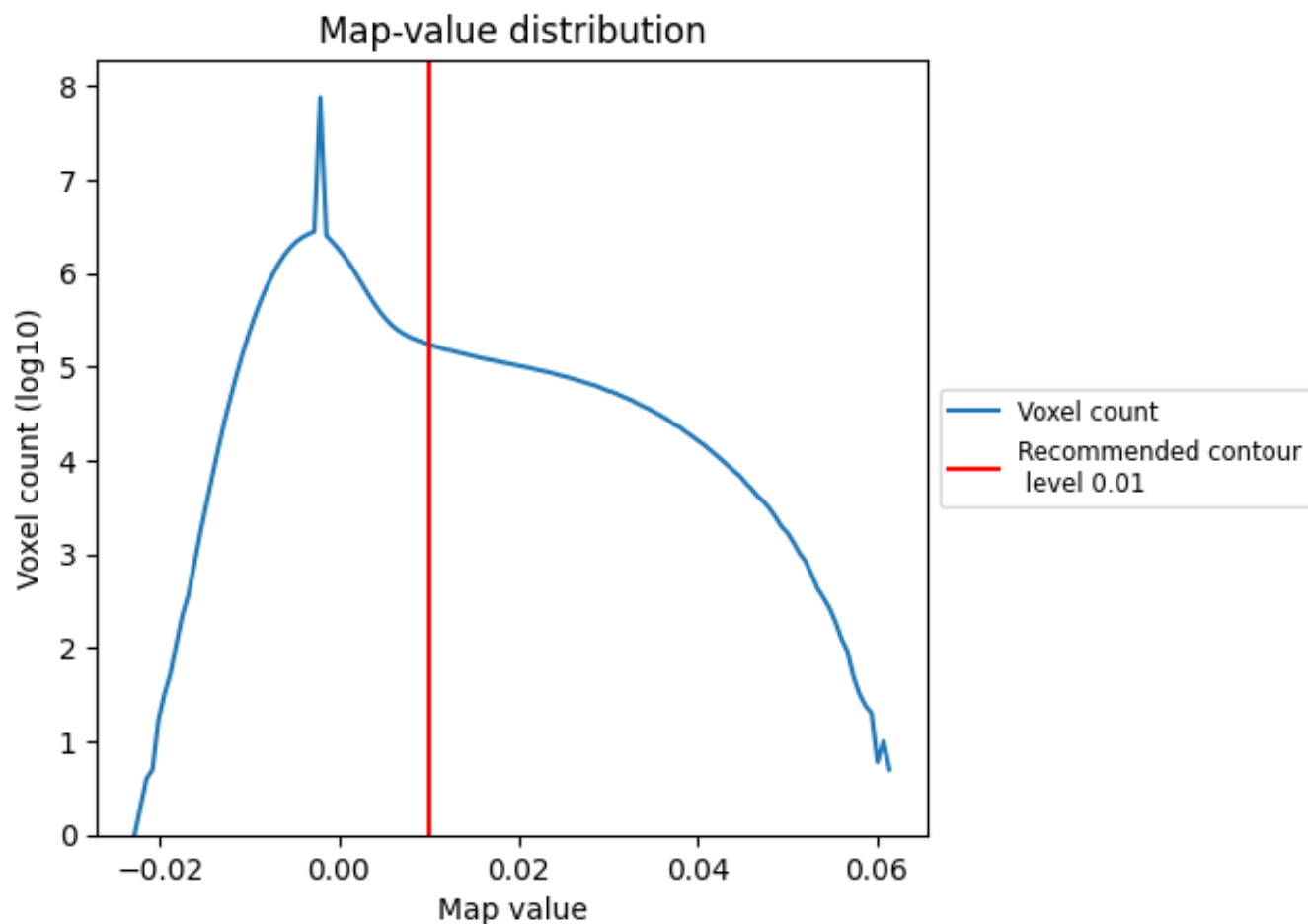
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

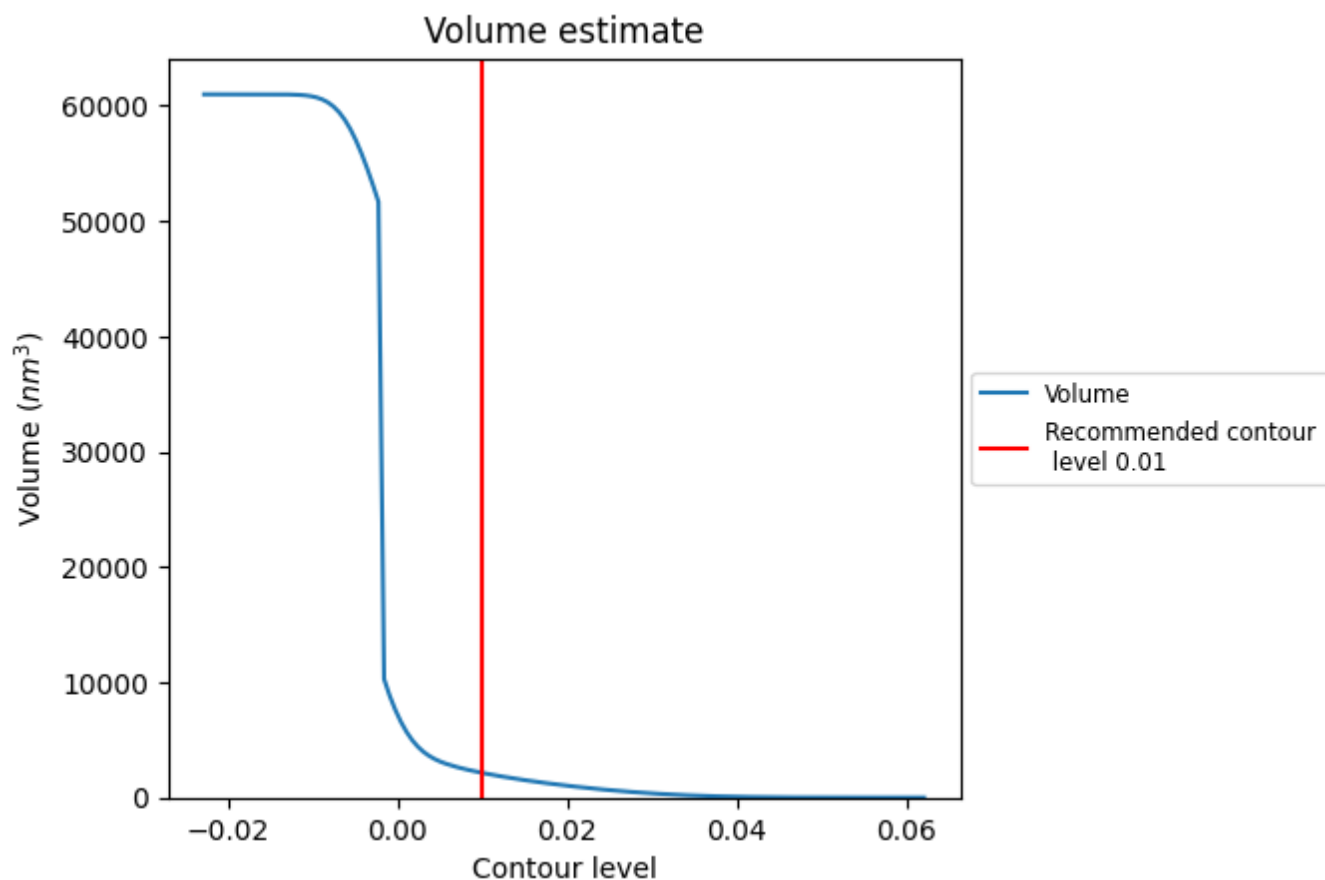
This section contains the results of statistical analysis of the map.

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



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

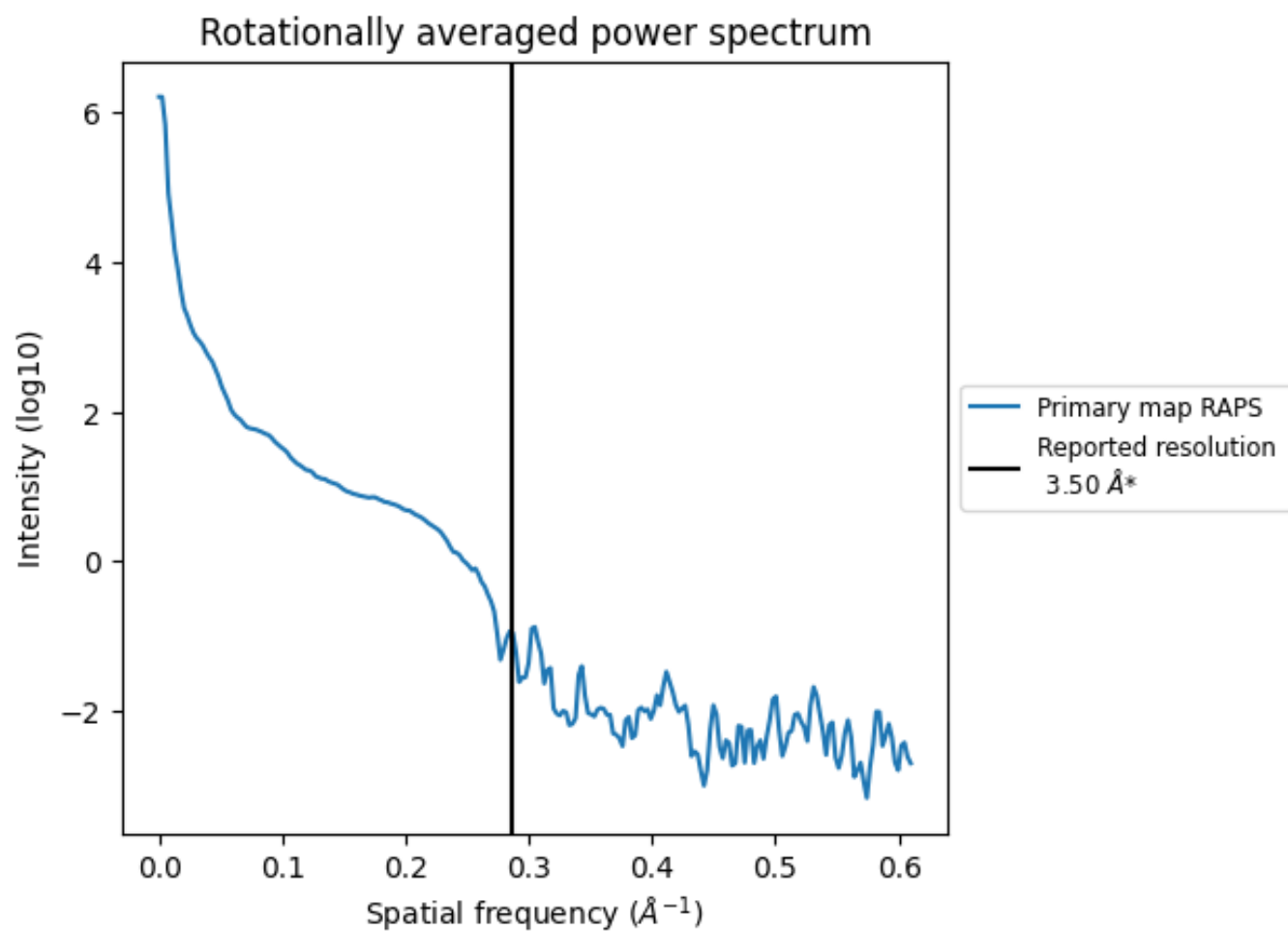
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2139 nm<sup>3</sup>; this corresponds to an approximate mass of 1932 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 0.286 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

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

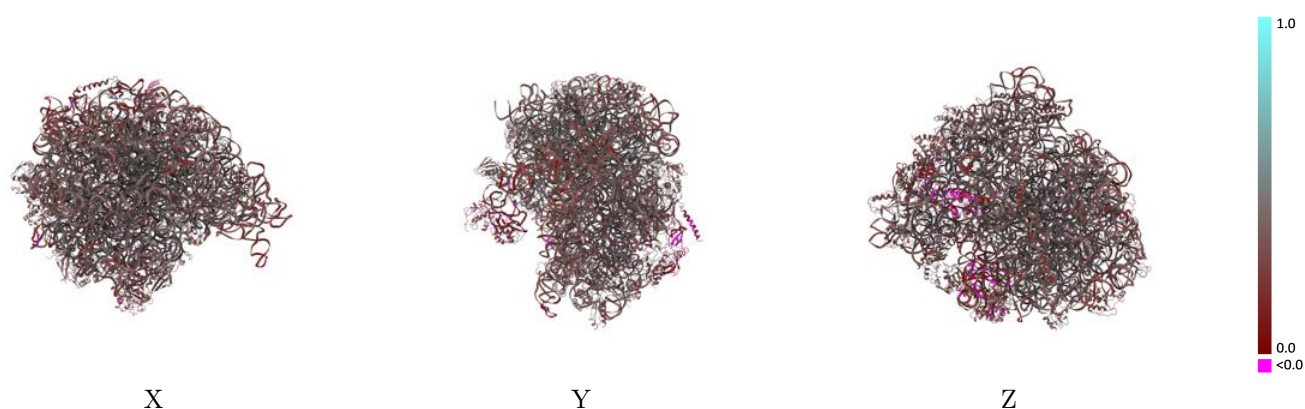
## 9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-7289 and PDB model 6BU8. Per-residue inclusion information can be found in section 3 on page 16.

### 9.1 Map-model overlay ⓘ

This section was not generated.

### 9.2 Q-score mapped to coordinate model ⓘ

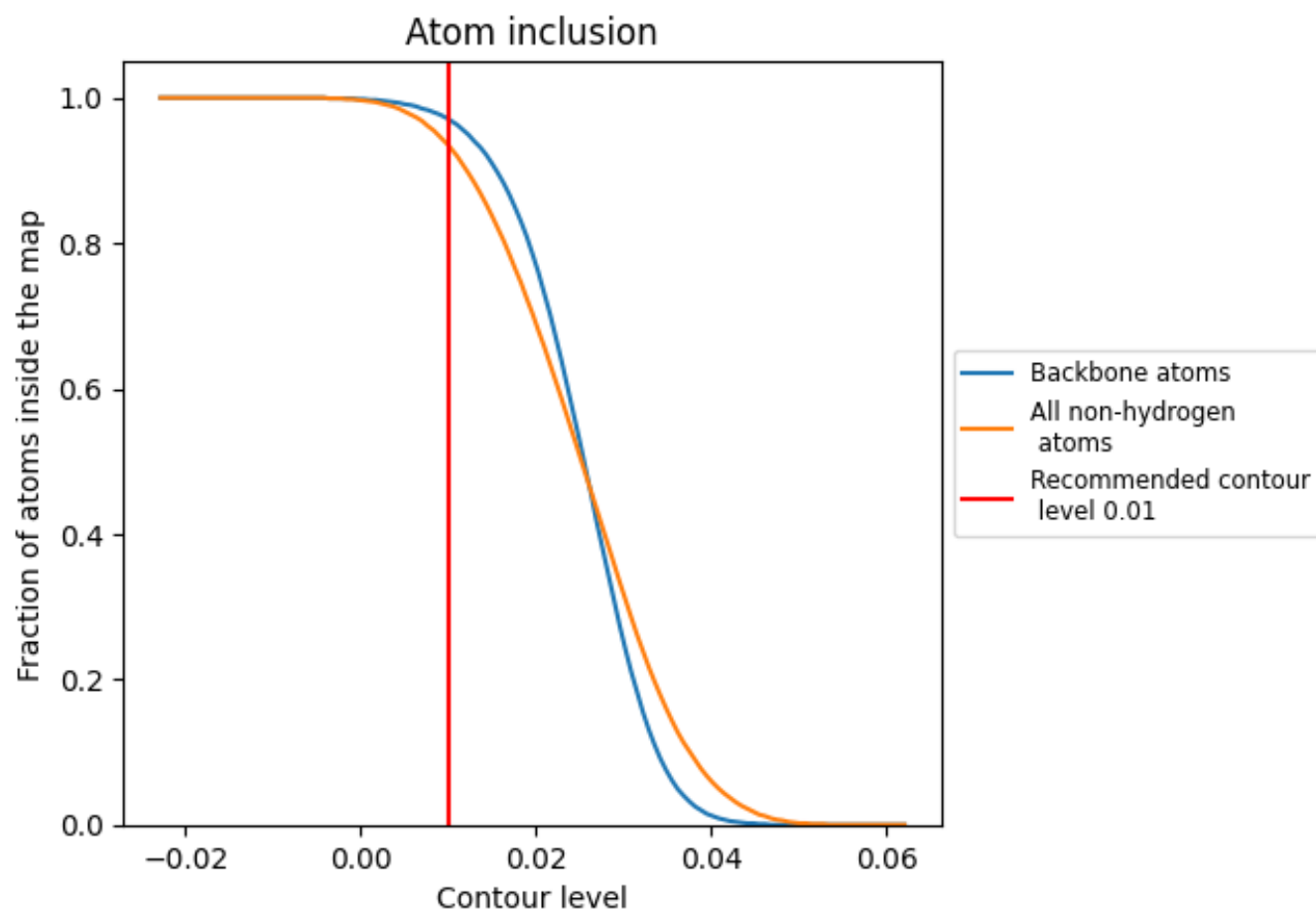


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

### 9.3 Atom inclusion mapped to coordinate model ⓘ

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9350   |  0.3600   |
| 01    |  0.9790   |  0.3740   |
| 02    |  0.9820   |  0.3500   |
| 03    |  0.8570   |  0.2350   |
| 04    |  0.8820   |  0.4170   |
| 05    |  0.8780   |  0.4050   |
| 06    |  0.8660   |  0.3690   |
| 07    |  0.8890   |  0.3370   |
| 08    |  0.8990   |  0.3530   |
| 09    |  0.7050   |  0.2910   |
| 10    |  0.5810   |  0.1830   |
| 11    |  0.6310   |  0.2060   |
| 12    |  0.8820   |  0.3750   |
| 13    |  0.8490   |  0.4110   |
| 14    |  0.8860  |  0.3910  |
| 15    |  0.8460 |  0.4040 |
| 16    |  0.9010 |  0.3760 |
| 17    |  0.9080 |  0.3530 |
| 18    |  0.8580 |  0.3900 |
| 19    |  0.8960 |  0.3830 |
| 20    |  0.8810 |  0.3820 |
| 21    |  0.8410 |  0.3890 |
| 22    |  0.8660 |  0.3670 |
| 23    |  0.9080 |  0.3540 |
| 24    |  0.8900 |  0.3790 |
| 25    |  0.9140 |  0.4020 |
| 26    |  0.8830 |  0.3980 |
| 27    |  0.8510 |  0.3030 |
| 28    |  0.9150 |  0.3890 |
| 29    |  0.8340 |  0.3230 |
| 30    |  0.9090 |  0.3970 |
| 31    |  0.8510 |  0.3810 |
| 32    |  0.8620 |  0.4010 |
| 33    |  0.8900 |  0.4120 |
| 34    |  0.9110 |  0.4000 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| A     |  0.9820   |  0.3640   |
| B     |  0.8730   |  0.3330   |
| C     |  0.8630   |  0.3740   |
| D     |  0.8850   |  0.3370   |
| E     |  0.8950   |  0.3830   |
| F     |  0.7180   |  0.2920   |
| G     |  0.8690   |  0.3430   |
| H     |  0.8820   |  0.3850   |
| I     |  0.8850   |  0.3570   |
| J     |  0.8410   |  0.3470   |
| K     |  0.8740   |  0.3790   |
| L     |  0.8680   |  0.3790   |
| M     |  0.9000   |  0.3420   |
| N     |  0.8880   |  0.3710   |
| O     |  0.8970   |  0.3520   |
| P     |  0.9200   |  0.3550   |
| Q     |  0.8770   |  0.3460   |
| R     |  0.9070   |  0.3730   |
| S     |  0.9160   |  0.3500   |
| T     |  0.8950  |  0.3300  |
| U     |  0.7740 |  0.3060 |
| V     |  0.8220 |  0.2680 |
| W     |  0.9350 |  0.3480 |
| X     |  0.8650 |  0.1800 |
| Y     |  0.9010 |  0.2770 |
| Z     |  0.3090 |  0.0490 |