



## Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:03 AM UTC

PDB ID : 8UPR / pdb\_00008upr  
EMDB ID : EMD-42454  
Title : Escherichia coli transcription-translation coupled complex class A (TTC-A) containing RfaH bound to ops signal, mRNA with a 21 nt long spacer, and fMet-tRNAs in E-site and P-site of the ribosome  
Authors : Molodtsov, V.; Wang, C.; Ebright, R.H.  
Deposited on : 2023-10-23  
Resolution : 5.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

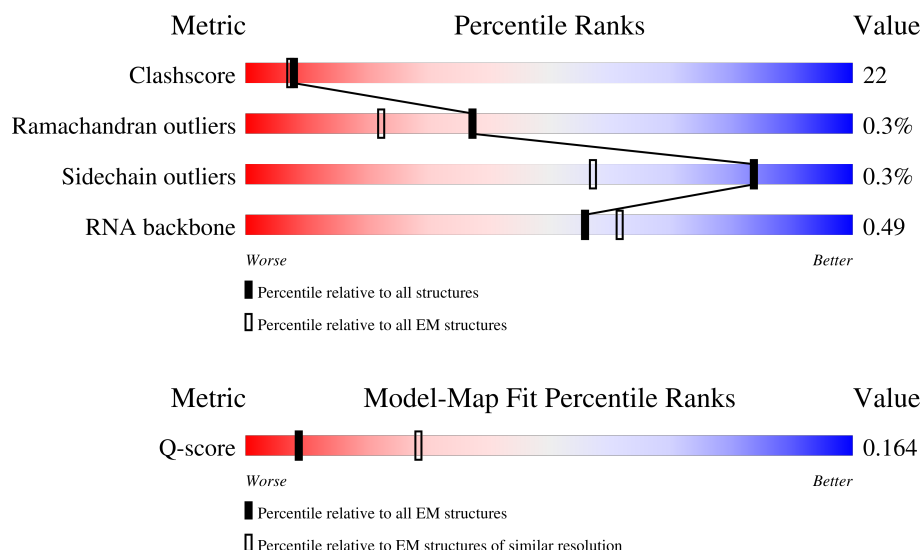
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 5.30 Å.

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



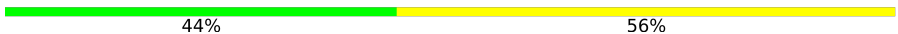
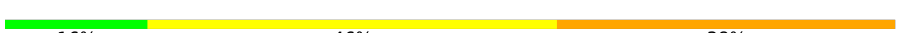
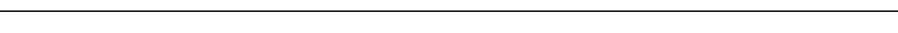
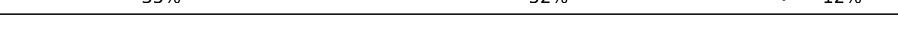
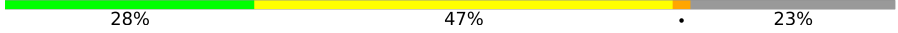
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 625 ( 4.80 - 5.80 )                                      |

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

| Mol | Chain | Length | Quality of chain                                         |
|-----|-------|--------|----------------------------------------------------------|
| 1   | 0     | 103    | <div> <div>59%</div> <div>41%</div> </div>               |
| 2   | 1     | 110    | <div> <div>59%</div> <div>41%</div> </div>               |
| 3   | 2     | 100    | <div> <div>51%</div> <div>42%</div> <div>6%</div> </div> |

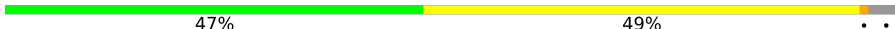
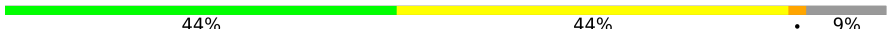
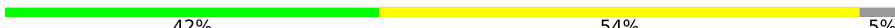
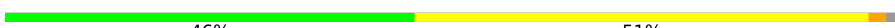
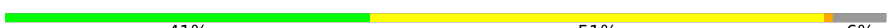
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | 3     | 104    |    |
| 5   | 4     | 94     |    |
| 6   | 5     | 38     |    |
| 7   | 6     | 38     |    |
| 8   | 7     | 38     |    |
| 9   | 9     | 165    |    |
| 10  | A     | 76     |    |
| 10  | B     | 76     |    |
| 11  | AA    | 1342   |    |
| 12  | AB    | 162    |    |
| 13  | AC    | 329    |    |
| 13  | AD    | 329    |    |
| 14  | AE    | 1407   |  |
| 15  | AF    | 91     |  |
| 16  | C     | 75     |  |
| 17  | D     | 1542   |  |
| 18  | E     | 87     |  |
| 19  | F     | 71     |  |
| 20  | G     | 241    |  |
| 21  | H     | 557    |  |
| 22  | I     | 233    |  |
| 23  | J     | 206    |  |
| 24  | K     | 167    |  |
| 25  | L     | 135    |  |
| 26  | M     | 179    |  |

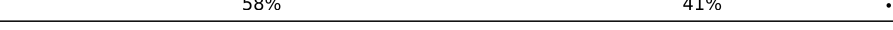
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 27  | N     | 130    |    |
| 28  | O     | 130    |    |
| 29  | P     | 103    |    |
| 30  | Q     | 129    |    |
| 31  | R     | 124    |    |
| 32  | S     | 101    |    |
| 33  | T     | 89     |    |
| 34  | U     | 82     |    |
| 35  | V     | 84     |    |
| 36  | W     | 92     |    |
| 37  | X     | 118    |    |
| 38  | Y     | 142    |   |
| 39  | Z     | 121    |  |
| 40  | a     | 2904   |  |
| 41  | b     | 85     |  |
| 42  | c     | 78     |  |
| 43  | d     | 120    |  |
| 44  | e     | 63     |  |
| 45  | f     | 59     |  |
| 46  | g     | 70     |  |
| 47  | h     | 273    |  |
| 48  | i     | 57     |  |
| 49  | j     | 209    |  |
| 50  | k     | 55     |  |
| 51  | l     | 201    |  |

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| Mol | Chain | Length | Quality of chain                                                                                |
|-----|-------|--------|-------------------------------------------------------------------------------------------------|
| 52  | m     | 46     |  57% 43%      |
| 53  | n     | 179    |  44% 54% ...  |
| 54  | o     | 65     |  58% 35% 5% . |
| 55  | p     | 177    |  68% 31% .    |
| 56  | q     | 38     |  61% 39%      |
| 57  | r     | 149    |  68% 32%      |
| 58  | s     | 142    |  55% 44% ..   |
| 59  | t     | 123    |  46% 54% .    |
| 60  | u     | 144    |  62% 37% .    |
| 61  | v     | 136    |  49% 49% .    |
| 62  | w     | 127    |  44% 46% . 6% |
| 63  | x     | 117    |  63% 36% .   |
| 64  | y     | 115    |  63% 37% .  |
| 65  | z     | 118    |  58% 41% .. |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 67  | ZN   | AE    | 1502 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 67 unique types of molecules in this entry. The entry contains 276059 atoms, of which 98639 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 Ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 1   | 0     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1655  | 516 | 839 | 153 | 145 | 2 |         |       |

- Molecule 2 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 2   | 1     | 110      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1779  | 532 | 922 | 166 | 156 | 3 |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 3   | 2     | 94       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1557  | 470 | 811 | 140 | 134 | 2 |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|--|---------|-------|
| 4   | 3     | 103      | Total | C   | H   | N   | O   |  | 0       | 0     |
|     |       |          | 1632  | 498 | 844 | 148 | 142 |  |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 5   | 4     | 94       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1533  | 479 | 780 | 137 | 134 | 3 |         |       |

- Molecule 6 is a DNA chain called NT DNA ops.

| Mol | Chain | Residues | Atoms |     |     |     |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|--|---------|-------|
| 6   | 5     | 35       | Total | C   | N   | O   | P  |  | 0       | 0     |
|     |       |          | 726   | 342 | 141 | 208 | 35 |  |         |       |

- Molecule 7 is a DNA chain called T DNA ops.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7   | 6     | 35       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 703   | 336 | 117 | 215 | 35 |         |       |

- Molecule 8 is a RNA chain called mRNA with 21 nt long spacer.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 8   | 7     | 38       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 792   | 354 | 112 | 288 | 38 |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | 9     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1117  | 705 | 196 | 209 | 7 |         |       |

- Molecule 10 is a RNA chain called E-site and P-site tRNA (fMet).

| Mol | Chain | Residues | Atoms         |          |          |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|----------|---------|---------|-------|
| 10  | A     | 76       | Total<br>2446 | C<br>723 | H<br>826 | N<br>295 | O<br>527 | P<br>75 | 0       | 0     |
| 10  | B     | 76       | Total<br>2434 | C<br>723 | H<br>814 | N<br>295 | O<br>527 | P<br>75 | 0       | 0     |

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 11  | AA    | 1316     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10381 | 6514 | 1810 | 2014 | 43 |         |       |

- Molecule 12 is a protein called Transcription antitermination protein RfaH.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | AB    | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1286  | 828 | 222 | 232 | 4 |         |       |

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | AC    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1698  | 1060 | 299 | 333 | 6 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | AD    | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1677  | 1048 | 297 | 326 | 6 |         |       |

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 14  | AE    | 1337     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10404 | 6535 | 1856 | 1963 | 50 |         |       |

- Molecule 15 is a protein called DNA-directed RNA polymerase subunit omega.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | AF    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 650   | 396 | 122 | 131 | 1 |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 16  | C     | 66       | Total | C   | H   | N   | O  | S       |       |
|     |       |          | 1103  | 344 | 559 | 102 | 97 | 1       | 0     |

- Molecule 17 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |       |      |       | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|------|-------|---------|-------|
| 17  | D     | 1524     | Total | C     | H     | N    | O     | P       |       |
|     |       |          | 49126 | 14585 | 16423 | 6003 | 10591 | 1524    | 0     |

- Molecule 18 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|-------|
| 18  | E     | 86       | Total | C   | H   | N   | O   | S       |       |
|     |       |          | 1388  | 414 | 719 | 138 | 114 | 3       | 0     |

- Molecule 19 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 19  | F     | 70       | Total | C   | H   | N   | O  | S       |       |
|     |       |          | 1218  | 366 | 629 | 125 | 97 | 1       | 0     |

- Molecule 20 is a protein called 30S ribosomal protein S2.



| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 20  | G     | 225      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3545  | 1113 | 1785 | 316 | 323 | 8 |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S1.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 21  | H     | 259      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3184  | 1073 | 1454 | 305 | 349 | 3 |         |       |

- Molecule 22 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 22  | I     | 208      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3346  | 1036 | 1710 | 307 | 290 | 3 |         |       |

- Molecule 23 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 23  | J     | 205      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3350  | 1026 | 1707 | 315 | 298 | 4 |         |       |

- Molecule 24 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 24  | K     | 156      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2348  | 717 | 1196 | 217 | 212 | 6 |         |       |

- Molecule 25 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 25  | L     | 104      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1694  | 536 | 846 | 153 | 152 | 7 |         |       |

- Molecule 26 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 26  | M     | 151      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2416  | 735 | 1235 | 227 | 215 | 4 |         |       |

- Molecule 27 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 27  | N     | 129      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2010  | 616 | 1031 | 173 | 184 | 6 |         |       |

- Molecule 28 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 28  | O     | 127      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2092  | 634 | 1070 | 206 | 179 | 3 |         |       |

- Molecule 29 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 29  | P     | 99       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1621  | 495 | 831 | 151 | 143 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 30  | Q     | 117      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1764  | 540 | 887 | 174 | 160 | 3 |         |       |

- Molecule 31 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 31  | R     | 121      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 1940  | 580 | 1001 | 194 | 161 | 4 |         |       |

- Molecule 32 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 32  | S     | 100      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 499 | 844 | 164 | 139 | 3 |         |       |

- Molecule 33 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 33  | T     | 88       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1448  | 439 | 734 | 144 | 130 | 1 |         |       |

- Molecule 34 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 34  | U     | 82       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1315  | 406 | 666 | 128 | 114 | 1 |         |       |

- Molecule 35 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 35  | V     | 80       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1339  | 411 | 691 | 121 | 113 | 3 |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 36  | W     | 83       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1351  | 424 | 688 | 126 | 111 | 2 |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 37  | X     | 116      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1864  | 558 | 964 | 181 | 158 | 3 |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | Y     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L7/L12.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 39  | Z     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 227   | 144 | 33 | 47 | 3 |         |       |

- Molecule 40 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|-------|------|---------|-------|
| 40  | a     | 2880     | Total | C     | H     | N     | O     | P    | 0       | 0     |
|     |       |          | 92918 | 27587 | 31077 | 11398 | 19976 | 2880 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference    |
|-------|---------|----------|--------|----------|--------------|
| a     | 887     | A        | U      | conflict | GB 937521852 |

- Molecule 41 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 41  | b     | 76       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1181  | 360 | 599 | 117 | 104 | 1 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 42  | c     | 77       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1277  | 388 | 652 | 129 | 106 | 2 |         |       |

- Molecule 43 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|-----|---------|-------|
| 43  | d     | 120      | Total | C    | H    | N   | O   | P   | 0       | 0     |
|     |       |          | 3870  | 1144 | 1301 | 468 | 837 | 120 |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 44  | e     | 62       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1032  | 308 | 531 | 98 | 94 | 1 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 45  | f     | 58       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 936   | 281 | 488 | 87 | 78 | 2 |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 46  | g     | 66       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1042  | 323 | 520 | 99 | 94 | 6 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 47  | h     | 271      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4236  | 1288 | 2154 | 423 | 364 | 7 |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 48  | i     | 56       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 903   | 269 | 459 | 94 | 80 | 1 |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 49  | j     | 209      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3182  | 979 | 1617 | 288 | 294 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|--|---------|-------|
| 50  | k     | 52       | Total | C   | H   | N  | O  |  | 0       | 0     |
|     |       |          | 890   | 275 | 464 | 78 | 73 |  |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 51  | l     | 201      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3171  | 974 | 1619 | 283 | 290 | 5 |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 52  | m     | 46       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 795   | 228 | 418 | 90 | 57 | 2 |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 53  | n     | 177      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2853  | 899 | 1443 | 249 | 256 | 6 |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 54  | o     | 64       | Total | C   | H   | N   | O  | S | 0       | 0     |
|     |       |          | 1076  | 323 | 572 | 105 | 74 | 2 |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 55  | p     | 175      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2671  | 826 | 1358 | 241 | 244 | 2 |         |       |

- Molecule 56 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 56  | q     | 38       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 645   | 185 | 343 | 65 | 48 | 4 |         |       |

- Molecule 57 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 57  | r     | 149      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2259  | 699 | 1148 | 197 | 214 | 1 |         |       |

- Molecule 58 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 58  | s     | 142      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2291  | 714 | 1162 | 212 | 199 | 4 |         |       |

- Molecule 59 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 59  | t     | 123      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 1969  | 593 | 1023 | 181 | 166 | 6 |         |       |

- Molecule 60 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 60  | u     | 144      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2182  | 654 | 1129 | 207 | 190 | 2 |         |       |

- Molecule 61 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 61  | v     | 136      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2231  | 686 | 1157 | 205 | 177 | 6 |         |       |

- Molecule 62 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 62  | w     | 119      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1945  | 588 | 994 | 195 | 163 | 5 |         |       |

- Molecule 63 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|--|---------|-------|
| 63  | x     | 116      | Total | C   | H   | N   | O   |  | 0       | 0     |
|     |       |          | 1815  | 552 | 923 | 178 | 162 |  |         |       |

- Molecule 64 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 64  | y     | 114      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1879  | 574 | 962 | 179 | 163 | 1 |         |       |

- Molecule 65 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |      |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|--|---------|-------|
| 65  | z     | 117      | Total | C   | H    | N   | O   |  | 0       | 0     |
|     |       |          | 1967  | 604 | 1020 | 192 | 151 |  |         |       |

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 66  | AE    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

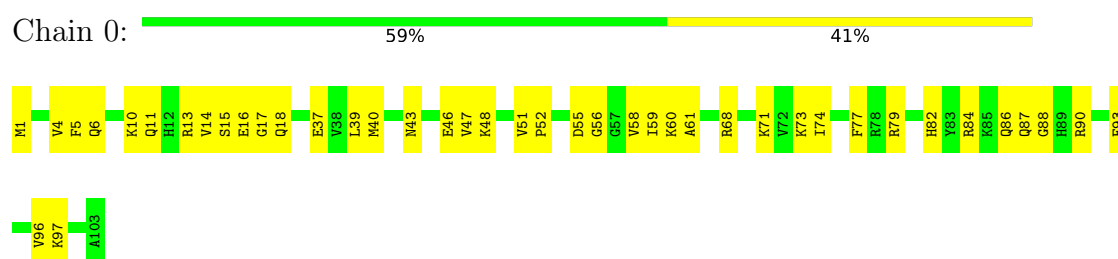
- Molecule 67 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 67  | AE    | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |

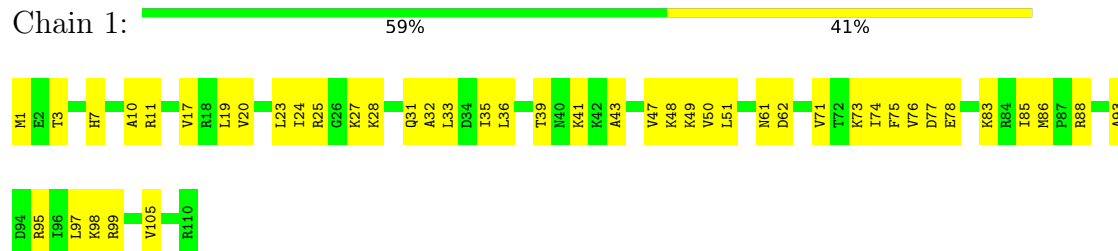
### 3 Residue-property plots

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.

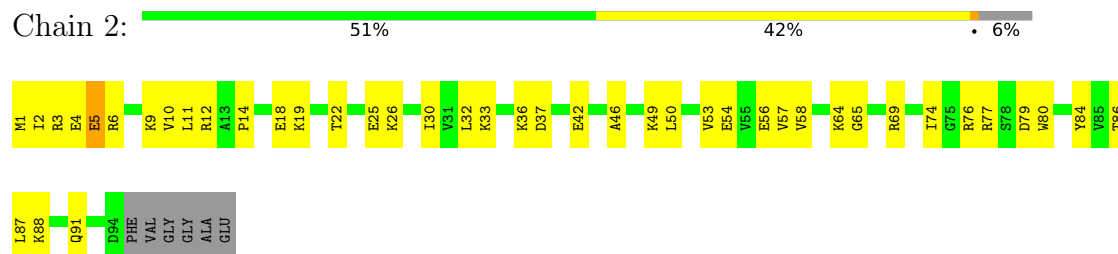
#### • Molecule 1: Ribosomal protein L21



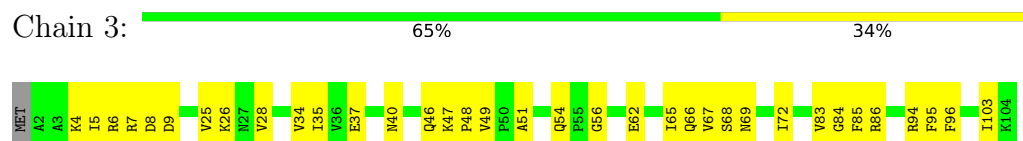
#### • Molecule 2: 50S ribosomal protein L22



#### • Molecule 3: 50S ribosomal protein L23

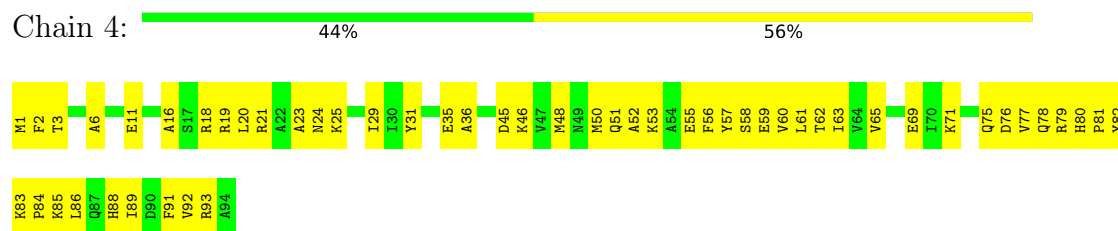


#### • Molecule 4: 50S ribosomal protein L24

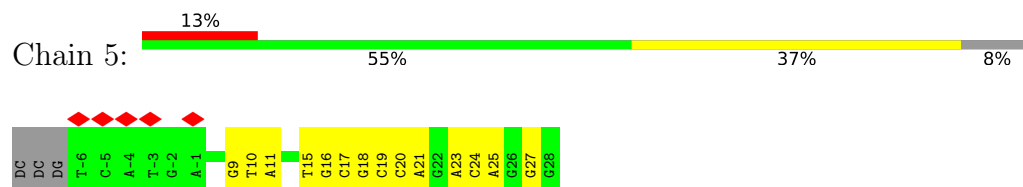




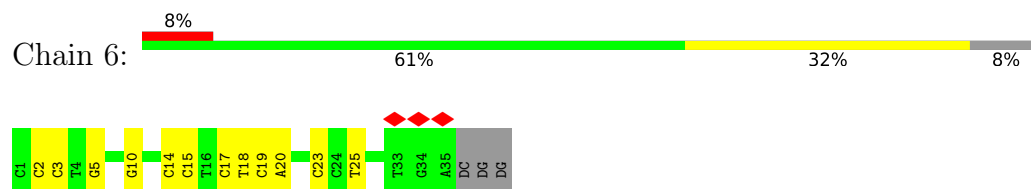
- Molecule 5: 50S ribosomal protein L25



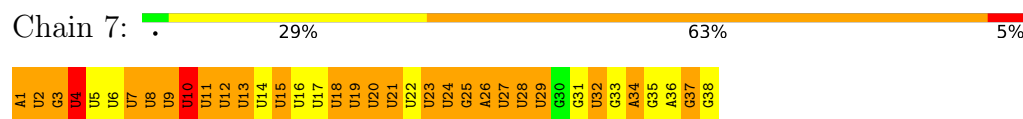
- Molecule 6: NT DNA ops



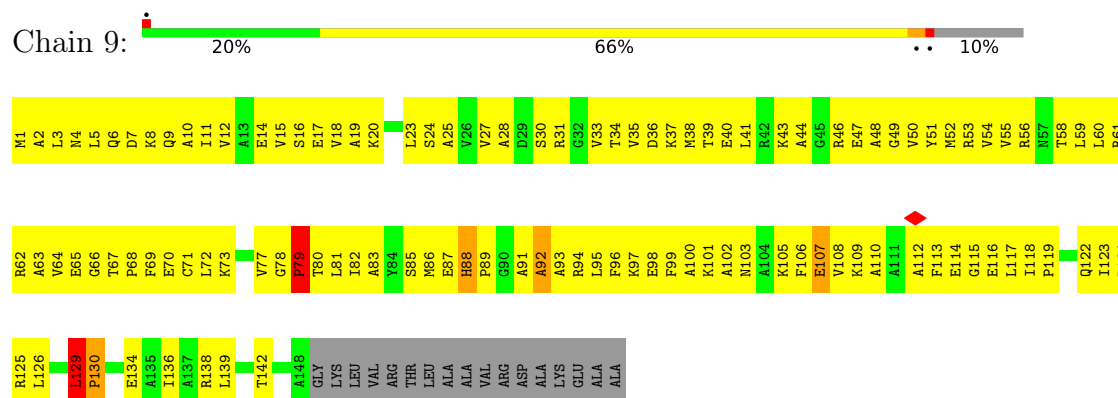
- Molecule 7: T DNA ops



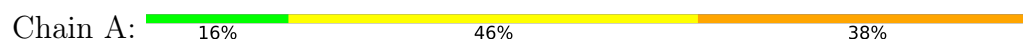
- Molecule 8: mRNA with 21 nt long spacer

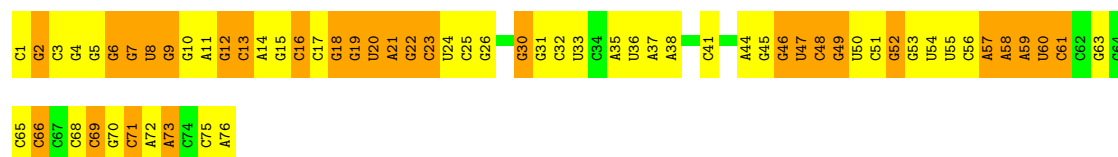


- Molecule 9: 50S ribosomal protein L10

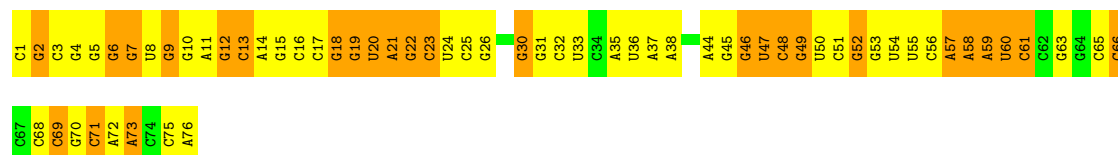
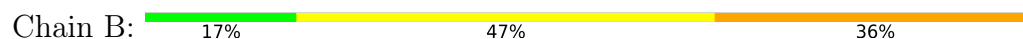


- Molecule 10: E-site and P-site tRNA (fMet)

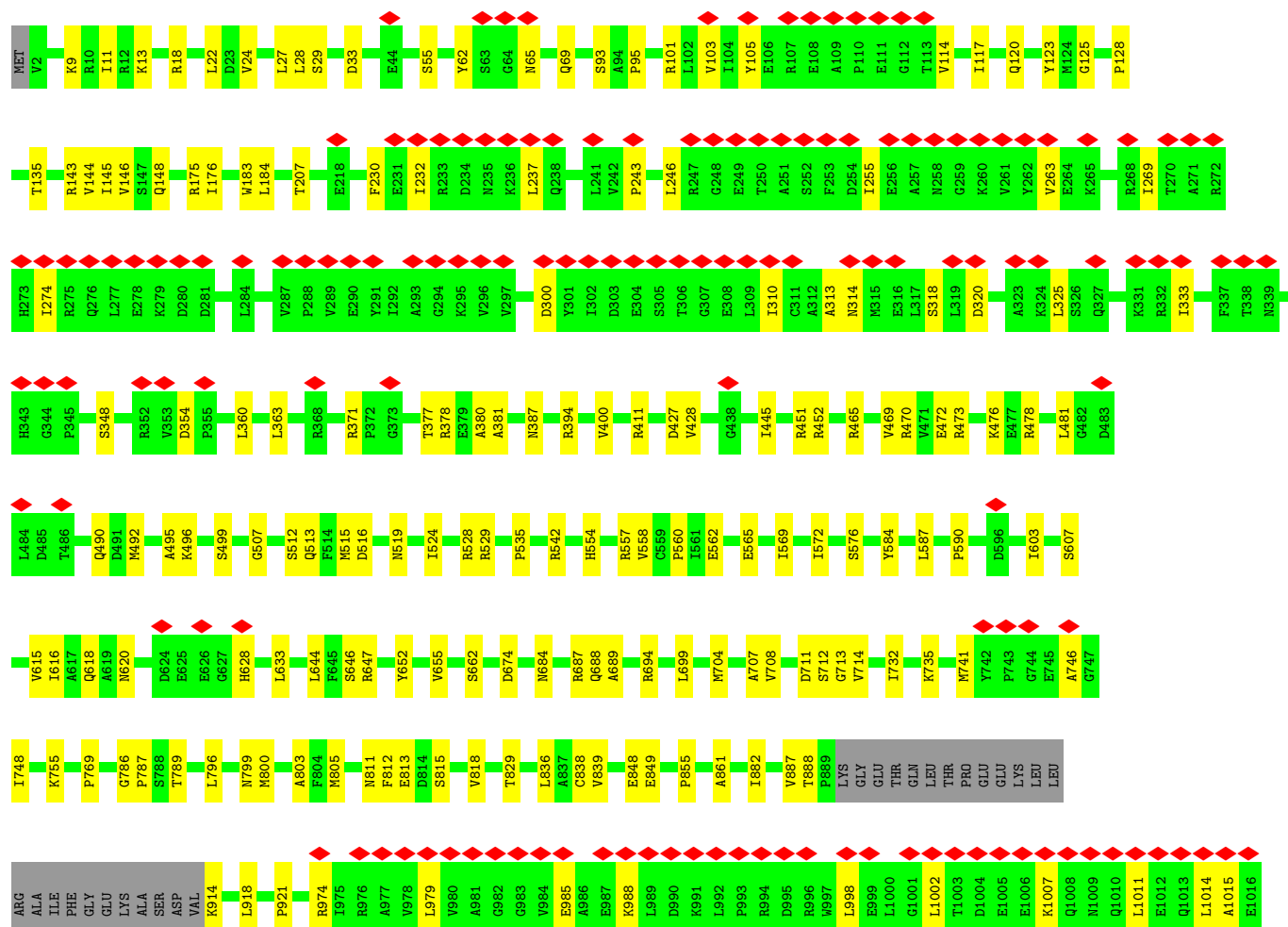
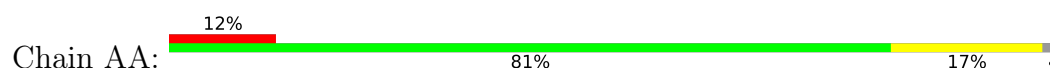




• Molecule 10: E-site and P-site tRNA (fMet)



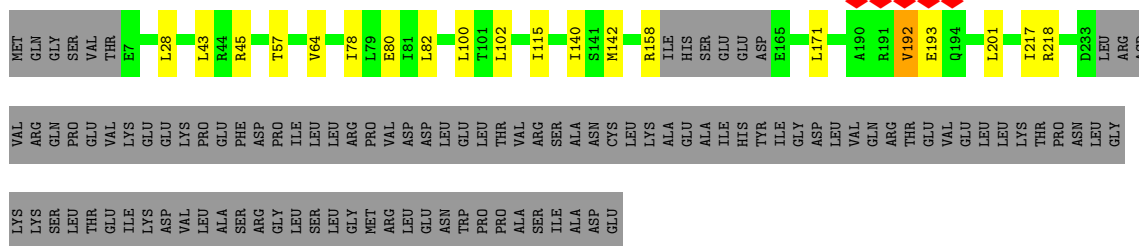
• Molecule 11: DNA-directed RNA polymerase subunit beta



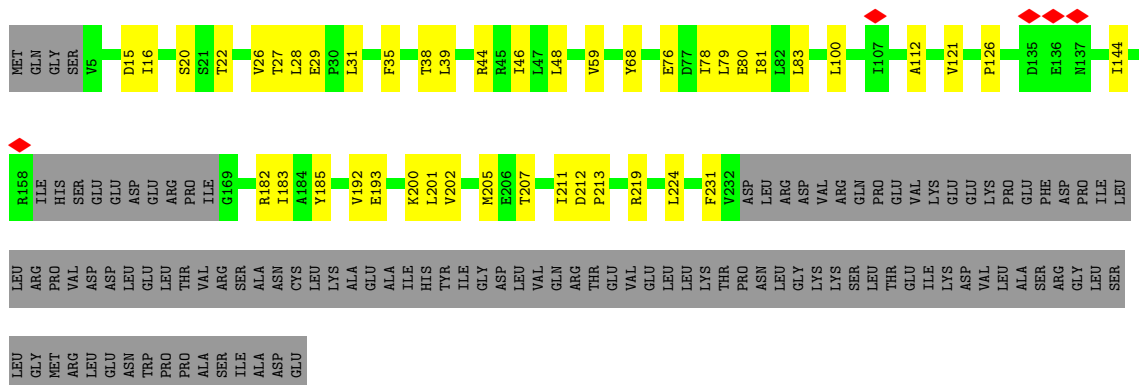
- Molecule 12: Transcription antitermination protein RfaH



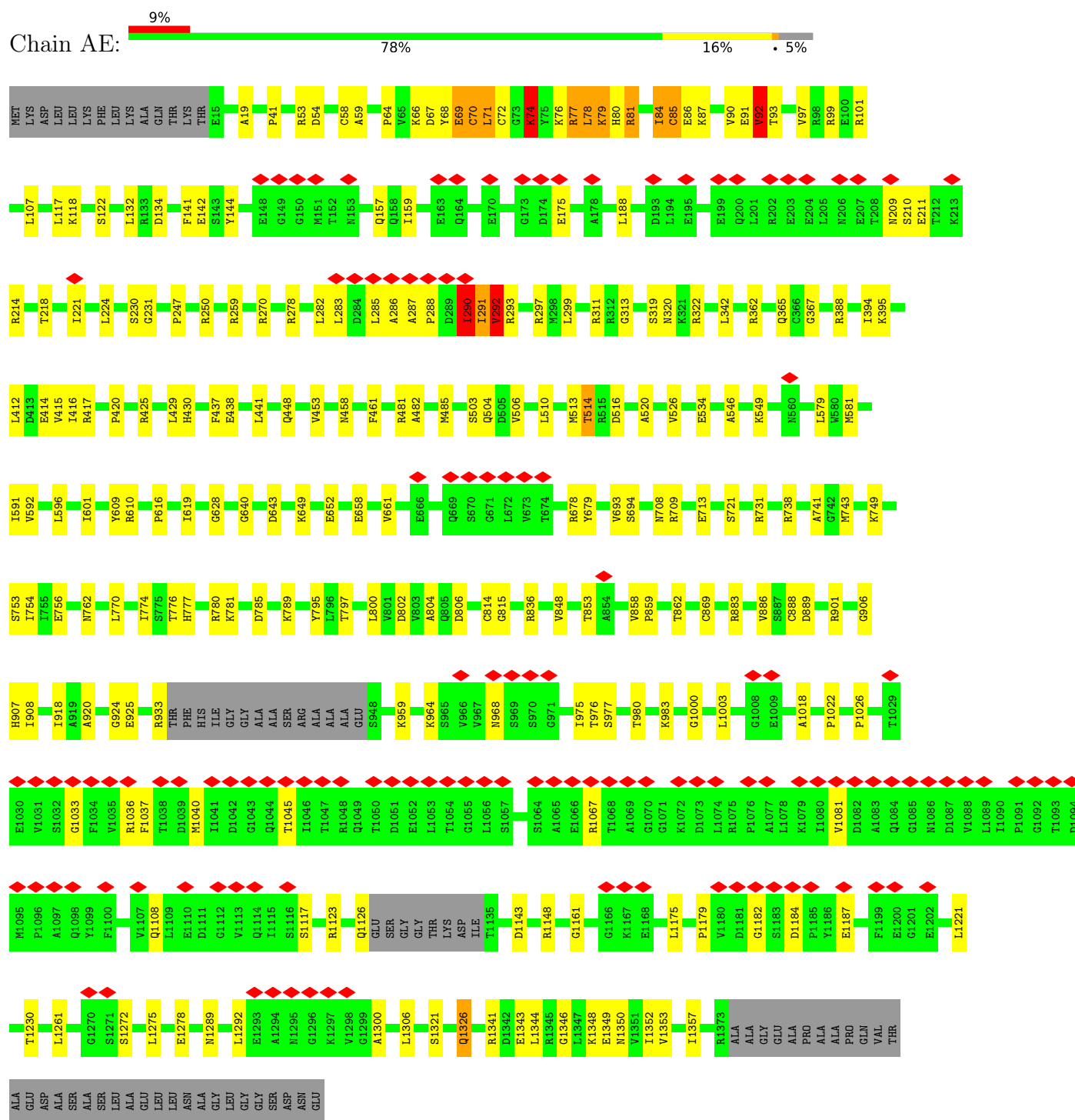
- Molecule 13: DNA-directed RNA polymerase subunit alpha



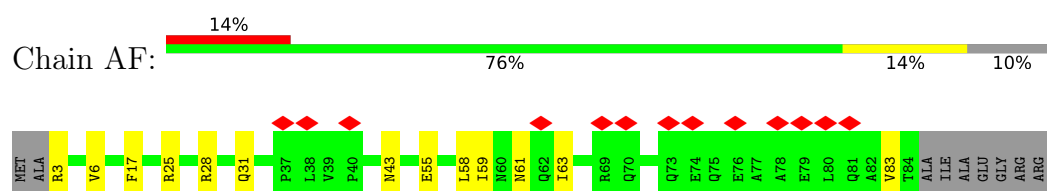
- Molecule 13: DNA-directed RNA polymerase subunit alpha



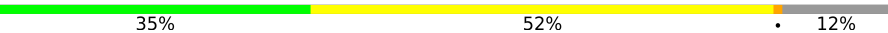
• Molecule 14: DNA-directed RNA polymerase subunit beta'



• Molecule 15: DNA-directed RNA polymerase subunit omega



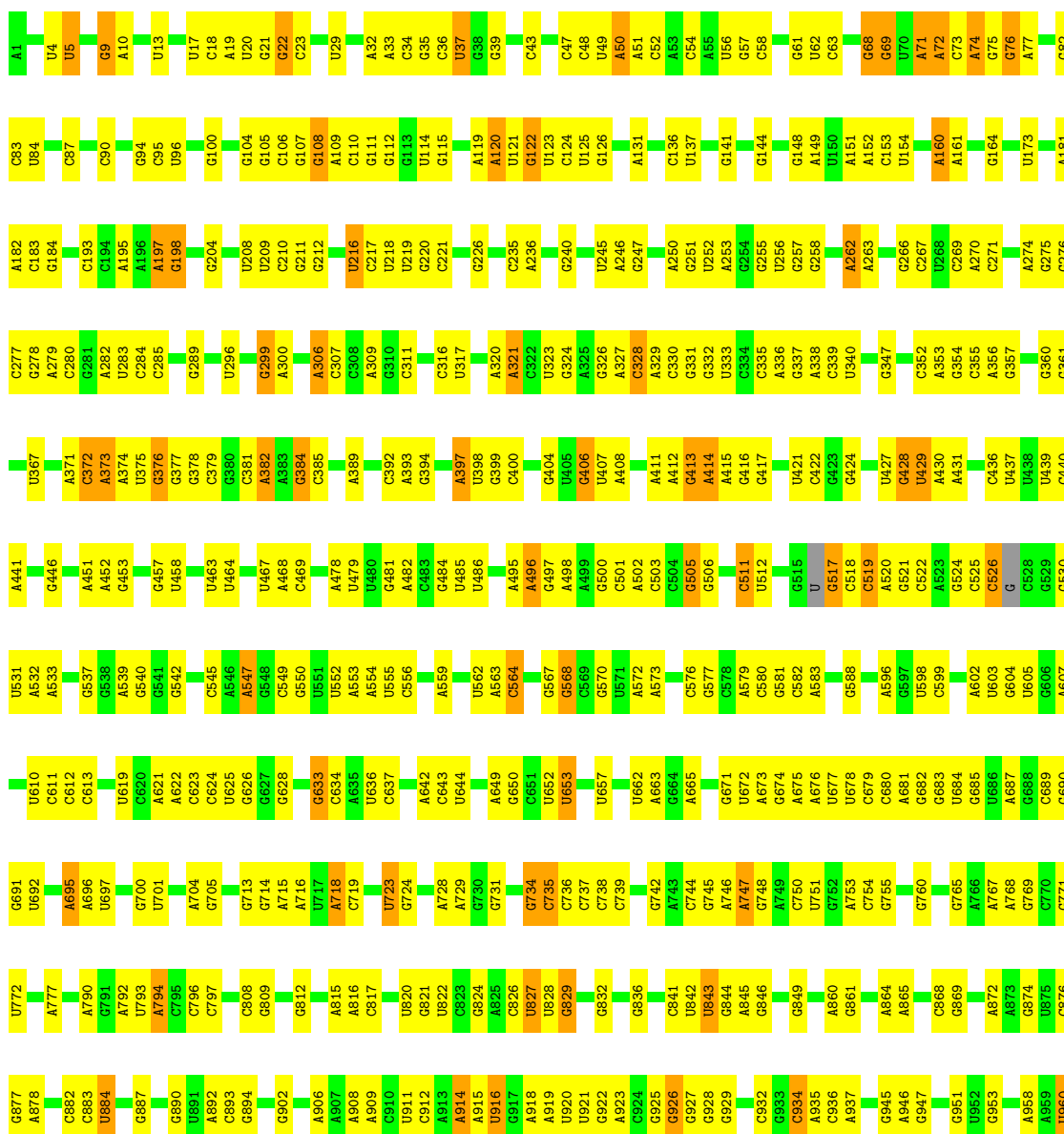
- Molecule 16: 30S ribosomal protein S18

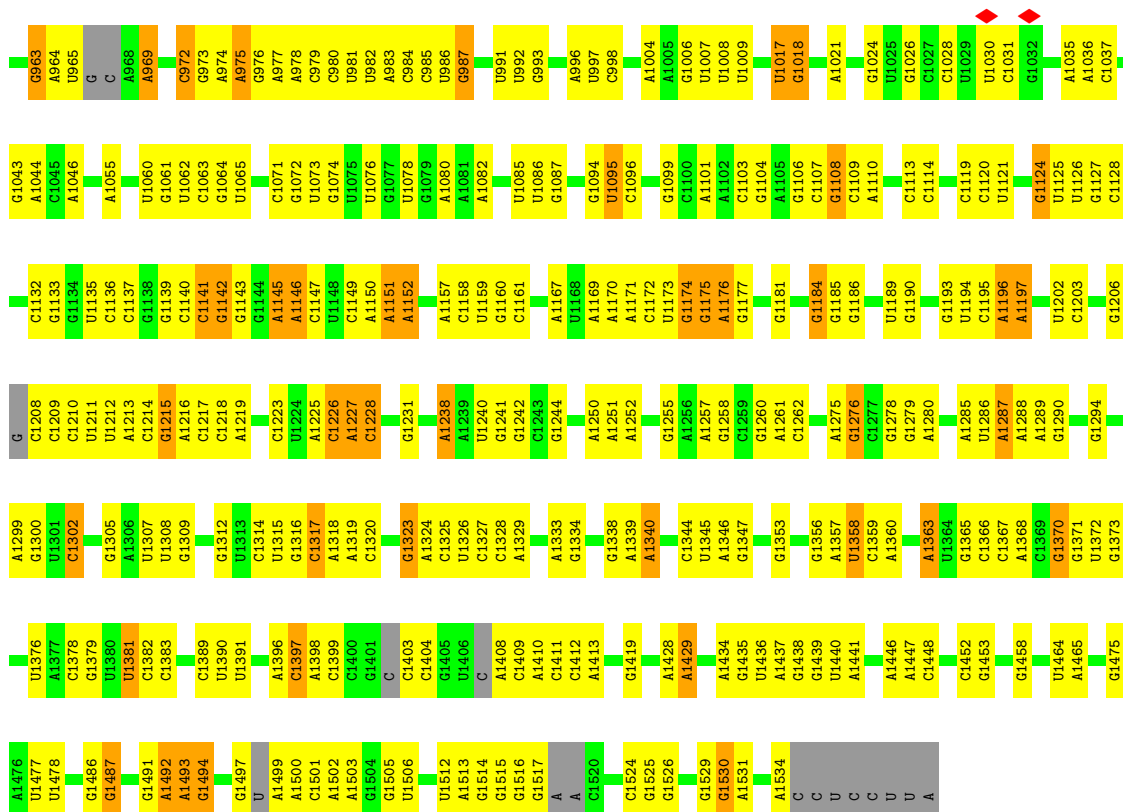
Chain C:  35% 52% 12%



- Molecule 17: 16S rRNA

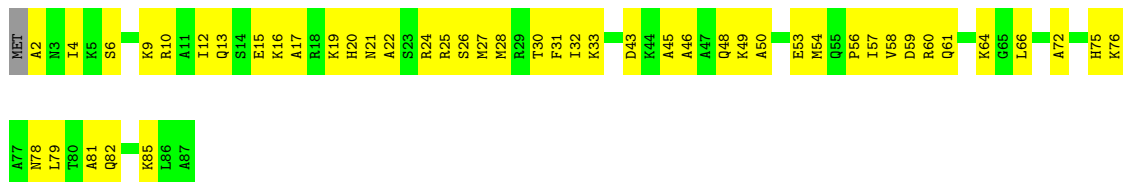
Chain D:  49% 43% 7%





• Molecule 18: 30S ribosomal protein S20

Chain E: 45% 54%



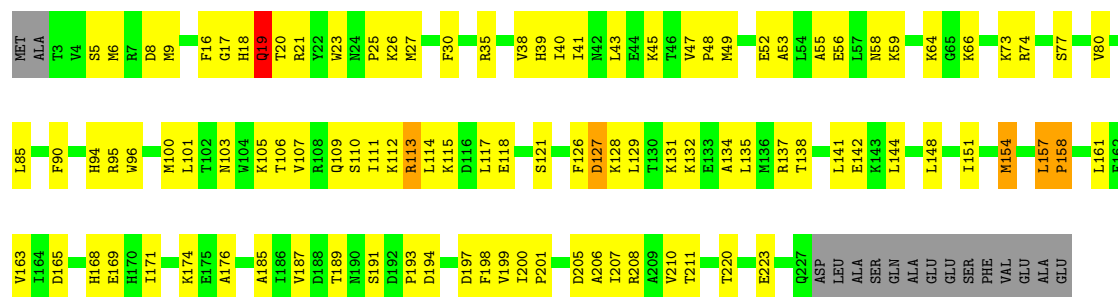
• Molecule 19: 30S ribosomal protein S21

Chain F: 41% 58%

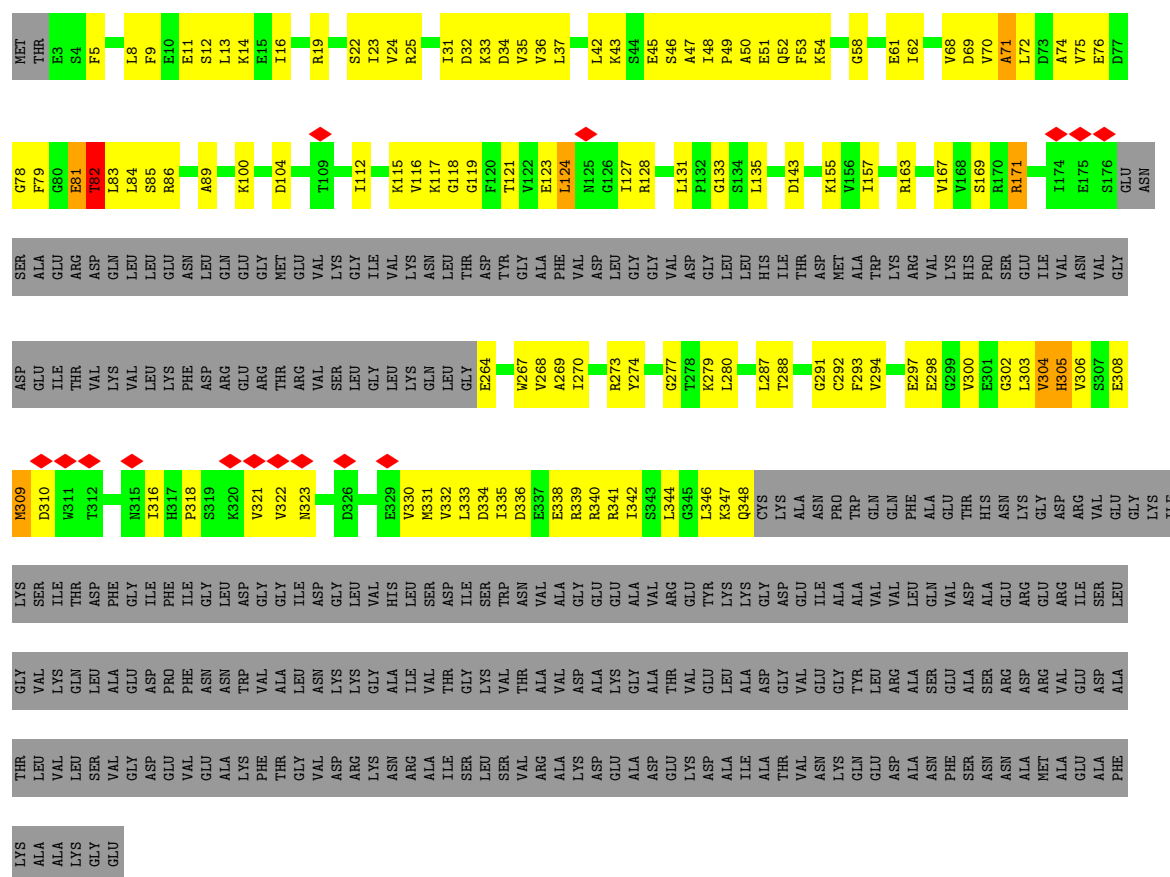


• Molecule 20: 30S ribosomal protein S2

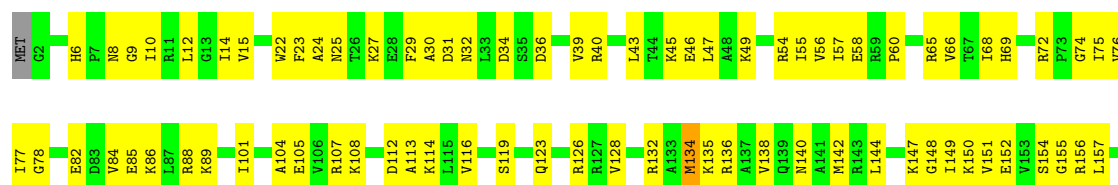
Chain G: 51% 40% 7%



• Molecule 21: 30S ribosomal protein S1

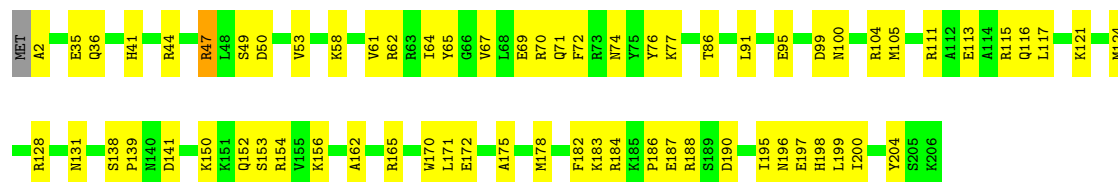


• Molecule 22: 30S ribosomal protein S3

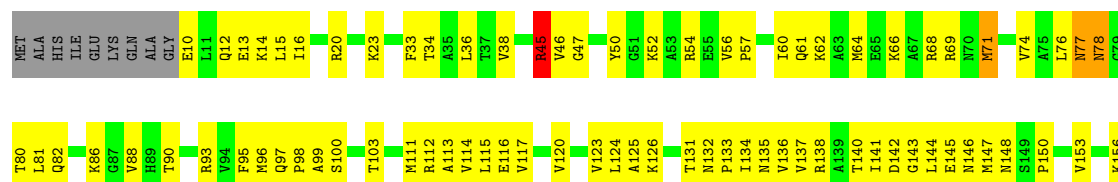




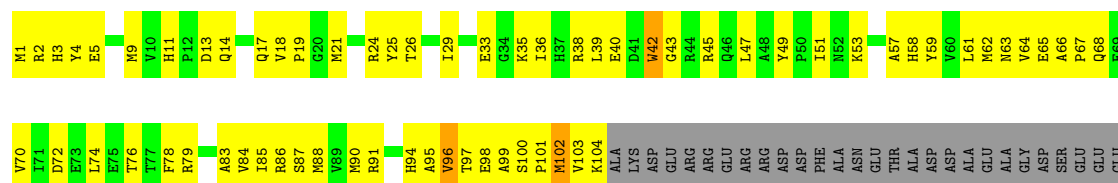
- Molecule 23: 30S ribosomal protein S4



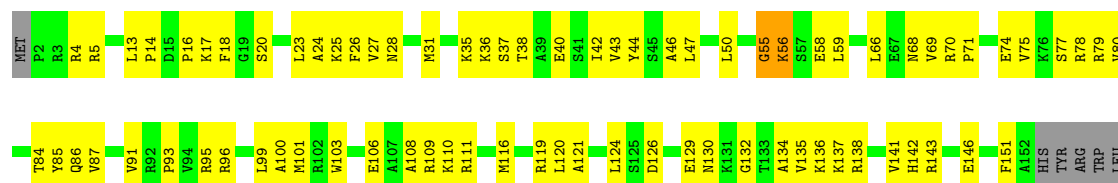
- Molecule 24: 30S ribosomal protein S5



- Molecule 25: 30S ribosomal protein S6



- Molecule 26: 30S ribosomal protein S7





SER  
LEU  
ARG  
SER  
PHE  
SER  
HIS  
GLN  
ALA  
GLY  
ALA  
SER  
SER  
LYS  
GLN  
PRO  
ALA  
LEU  
GLY  
TYR  
LEU  
ASN

• Molecule 27: 30S ribosomal protein S8

Chain N:  51% 48%

MET S2 M3 Q4 D5 P6 P6 I7 A8 D9 M10 L11 T12 R13 M16 A24 V25 T26 T27 P28 K31 L32 K33 V34 A35 V39 L40 E43 G44 E47 K50 V51 E52 G53 K56 P57 E58 L59 E60 L63 K64 Y65 F66 Q67 V71 R77 V78 R80

L83 R84 R85 Y86 K87 R88 K89 D90 L92 M96 L99 G100 I101 V104 S105 T106 V110 M111 T112 D113 R114 A115 L121 E124 I125 A130

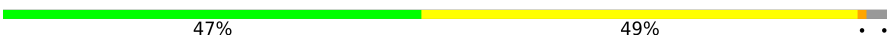
• Molecule 28: 30S ribosomal protein S9

Chain O:  49% 45%

MET ALA GLU N4 Y6 Y7 G8 T9 E89 G10 R11 R12 K13 F20 T21 K22 M25 G26 K27 T30 R31 Q32 L35 F39 G40 R41 A44 R45 M46 V47 V48 R49 Q50 P51 L52 E53 E55 D56 M57 V58 E59 K60 L63 Y64 T65 T66 V67 K68 G71 A78

I79 R80 T83 T84 R85 A86 L87 M88 E89 Y90 D91 E92 E93 L94 R95 S96 E97 L98 F103 E112 R113 Q114 K115 V116 G117 L118 R123 R124 F127 S128 K129 R130

• Molecule 29: 30S ribosomal protein S10

Chain P:  47% 49%

MET GLN ASN R5 I6 R7 L10 K11 A12 F13 D14 H15 I18 A21 T22 A23 E24 L25 V26 E27 T28 A29 K30 R37 I40 R45 K46 E47 L52 T53 H56 V57 N58 K59 D60 A61 R62 D63 Q64 Y65 E66 I67 H70 L71 R72 L73 V74 D75 P79

T80 E81 K82 D85 A86 L87 M88 R89 L90 D91 L92 A93 A94 D97 I100 S101 L102 G103

• Molecule 30: 30S ribosomal protein S11

Chain Q:  44% 44% 9%

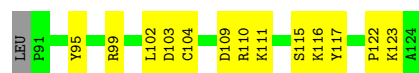
MET ALA LYS PRO ILE ARG ARG VAL K14 Q15 V20 A21 H22 T23 F27 I31 T34 T35 D36 N40 A41 L42 T46 T47 G48 G49 S50 G51 F52 R53 G54 S55 S56 F61 A62 A63 Q64 V65 D72 K75 E76 Y77 G78 I79 K80

E83 V84 M85 V86 K87 G88 P89 G90 P91 G92 G93 E94 S95 S96 T96 I97 R98 A99 L100 M101 F105 R106 I107 T108 M109 T110 T111 V113 T114 P115 T116 P117 H118 M119 P123 G124 P124 K125 K126 V129

• Molecule 31: 30S ribosomal protein S12

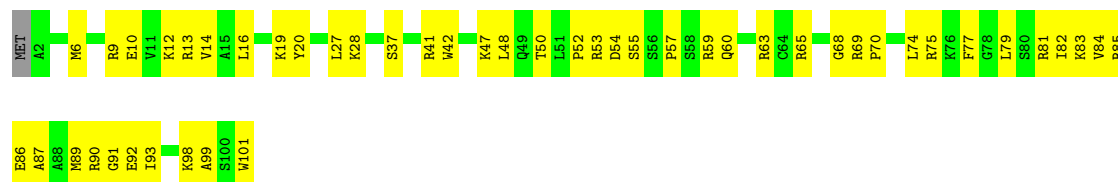
Chain R:  57% 40%

MET A2 T3 V4 N5 Q6 L7 V8 R9 R12 R13 A13 R14 K18 S19 S20 V21 P22 A23 L24 E25 C27 K30 R31 T35 Y38 T39 T40 R54 R55 V55 L57 T58 M59 E62 Y66 I67 G68 G69 E70 L74 Q75 V79 I80 L81 I82 R83 K88 ASP



- Molecule 32: 30S ribosomal protein S14

Chain S: 51% 48% .



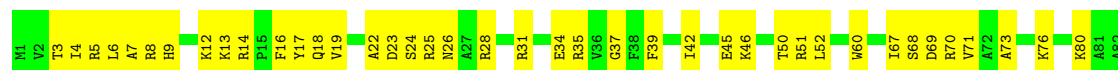
- Molecule 33: 30S ribosomal protein S15

Chain T: 42% 56% ..



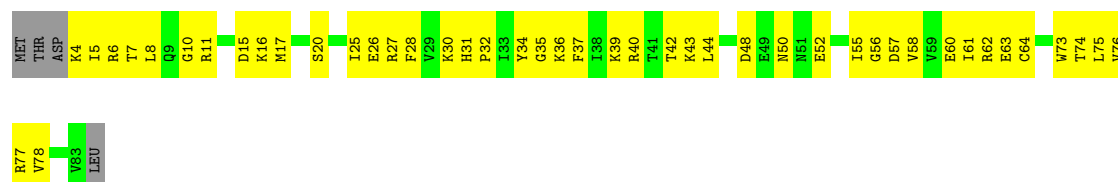
- Molecule 34: 30S ribosomal protein S16

Chain U: 51% 49%



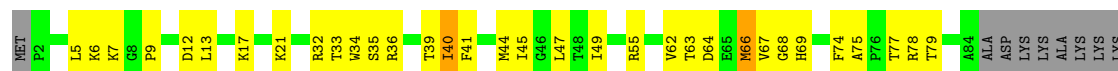
- Molecule 35: 30S ribosomal protein S17

Chain V: 42% 54% 5%

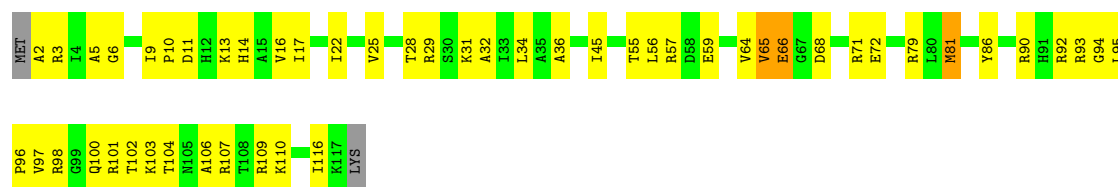


- Molecule 36: 30S ribosomal protein S19

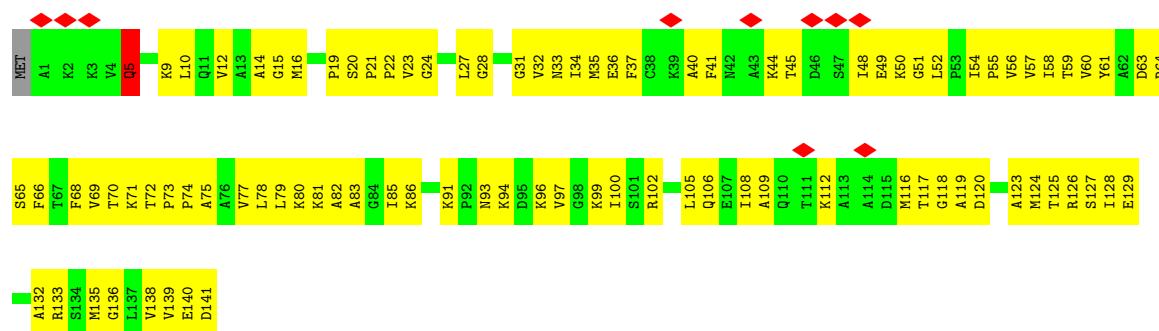
Chain W: 54% 34% 10%



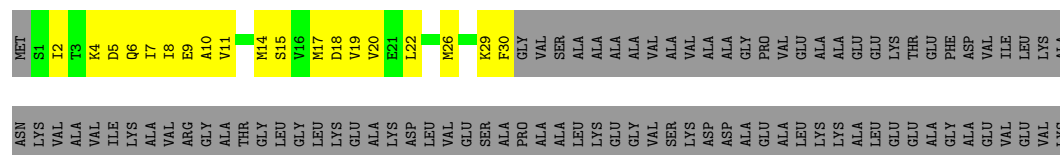
- Molecule 37: 30S ribosomal protein S13



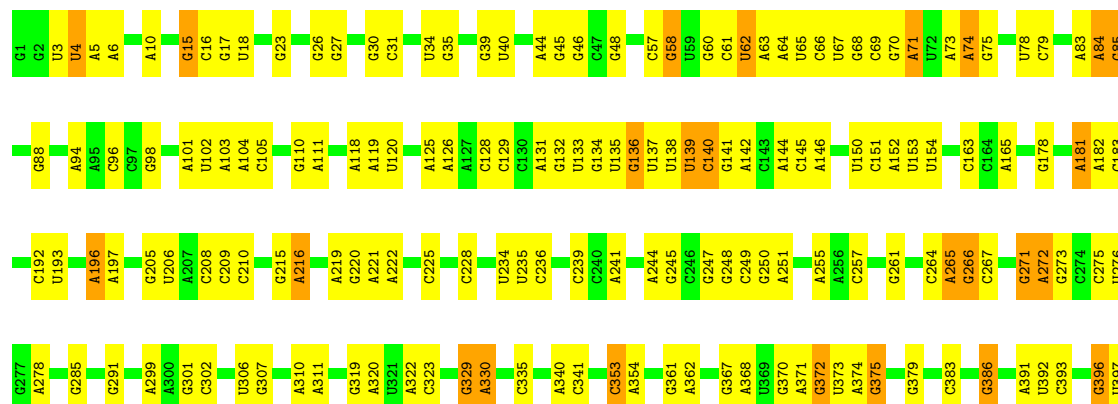
Chain Y:  7% 34% 65%



Chain Z:  9% 16% 75%



Chain a:  51% 41% 7%



|       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|
| G1613 | U1534 | G1421 | G1345 | G1250 | G1160 | A1080 | U1012 | G938  | G857 | G760 | U657 | G583 | A501 | C398 |
| A1614 | A1535 | G1422 | G1346 | C1251 | G1161 | U1081 | C1013 | G939  | G858 | G761 | U658 | C584 | A502 | U399 |
| C1536 | G1537 | A1427 | A1347 | A1252 | G1162 | U1082 | A1014 | G940  | U859 | A764 | G659 | G585 | A503 | G400 |
| A     | G1617 | C1428 | C1348 | A1253 | C1167 | U1083 | U1019 | A941  | G860 | G765 | A666 | C587 | A504 | U405 |
| G1619 | U1542 | G1429 | C1349 | G1256 | C1168 | A1084 | A1020 | A945  | G861 | A677 | A667 | U588 | A505 | A404 |
| G1622 | G1543 | G1430 | C1350 | C1257 | A1169 | A1085 | A1021 | C946  | G869 | U773 | A668 | U589 | C509 | G406 |
| U1647 | C1546 | A1431 | U1352 | A1262 | G1170 | A1086 | A1022 | C947  | U870 | G774 | G669 | A590 | G512 | G407 |
| U1648 | G1547 | G1432 | C1351 | G1266 | G1171 | A1087 | G1022 | C948  | U871 | G775 | A670 | U591 | G408 | G409 |
| G1649 | A1548 | A1433 | A1353 | U1267 | U1172 | A1088 | U1023 | C948  | U872 | G776 | U871 | U592 | G410 | G411 |
| A1550 | U1549 | G1434 | A1354 | G1268 | U1173 | A1089 | G1024 | C952  | U873 | G780 | C672 | U593 | G520 | G412 |
| G1651 | G1361 | G1435 | G1362 | A1269 | U1174 | A1090 | G1025 | G953  | G874 | A781 | A677 | C595 | U521 | A411 |
| U1554 | C1361 | G1441 | C1362 | C1270 | U1175 | A1095 | G1026 | G954  | U878 | A782 | U596 | A522 | C413 | C413 |
| A1652 | A1365 | G1442 | A1365 | G1271 | G1177 | A1096 | A1027 | U     | A879 | A783 | U597 | C523 | C414 | C414 |
| C1653 | U1443 | U1443 | A1453 | G1272 | A1272 | U1101 | A1028 | G956  | G878 | A784 | U598 | C523 | A415 | A415 |
| A1654 | G1444 | G1444 | G1445 | G1273 | G1179 | C1102 | A1029 | G957  | G880 | G785 | A599 | A529 | C420 | C420 |
| A1655 | G1368 | G1445 | G1369 | A1274 | U1180 | A1103 | U1033 | U958  | A689 | C786 | G600 | C531 | G424 | G424 |
| C1656 | G1370 | G1452 | G1371 | A1275 | U1181 | G1106 | G1036 | A960  | U884 | C787 | C601 | A532 | A432 | A432 |
| U1657 | A1378 | A1453 | G1371 | A1276 | U1182 | G1107 | G1037 | C961  | C885 | A789 | G700 | A532 | A443 | A443 |
| C1658 | G1379 | G1454 | A1383 | G1277 | U1183 | U1108 | G1038 | C962  | G888 | A800 | U702 | A532 | U427 | U427 |
| G1659 | A1386 | U1460 | C1380 | G1278 | G1186 | C1109 | G1039 | U963  | C889 | A800 | U703 | A532 | A432 | A432 |
| A1664 | C1386 | U1467 | G1387 | G1279 | G1187 | G1111 | A1040 | C964  | C890 | G805 | U704 | A532 | A432 | A432 |
| A1665 | C1387 | U1468 | A1387 | G1280 | G1188 | G1112 | G1041 | C965  | C891 | C806 | U705 | A532 | A432 | A432 |
| A1666 | C1388 | U1469 | A1388 | G1281 | U1189 | G1113 | G1042 | C966  | C892 | A807 | A706 | A532 | A432 | A432 |
| A1667 | C1389 | U1470 | A1389 | G1282 | G1190 | G1114 | G1043 | C967  | C893 | U807 | G707 | A532 | A432 | A432 |
| A1668 | C1390 | U1471 | A1390 | G1283 | C1196 | G1115 | G1044 | C968  | C894 | U811 | G708 | A532 | A432 | A432 |
| A1669 | C1391 | U1472 | A1391 | G1284 | G1197 | G1116 | G1045 | C969  | C895 | U812 | U709 | A532 | A432 | A432 |
| A1670 | C1392 | U1473 | A1392 | G1285 | G1198 | G1117 | G1046 | C970  | C896 | U813 | U710 | A532 | A432 | A432 |
| A1671 | C1393 | U1474 | A1393 | G1286 | G1199 | G1118 | G1047 | C971  | C897 | C814 | U711 | A532 | A432 | A432 |
| A1672 | C1394 | U1475 | A1394 | G1287 | G1200 | G1119 | G1048 | C972  | C898 | C815 | U712 | A532 | A432 | A432 |
| A1673 | C1395 | U1476 | A1395 | G1288 | U1201 | G1120 | G1049 | C973  | C899 | G818 | U713 | A532 | A432 | A432 |
| A1674 | C1396 | U1477 | A1396 | G1289 | A1204 | G1121 | C1053 | C974  | C900 | G819 | U714 | A532 | A432 | A432 |
| A1675 | C1397 | U1478 | A1397 | G1290 | A1205 | G1122 | G1054 | C975  | C901 | G820 | U715 | A532 | A432 | A432 |
| A1676 | C1398 | U1479 | A1398 | G1291 | A1206 | G1123 | G1055 | C976  | C902 | G821 | U716 | A532 | A432 | A432 |
| A1677 | C1399 | U1480 | A1399 | G1292 | G1206 | G1124 | G1056 | C977  | C903 | G822 | U717 | A532 | A432 | A432 |
| A1678 | C1400 | U1481 | A1400 | G1293 | G1207 | G1125 | G1057 | C978  | C904 | U823 | U718 | A532 | A432 | A432 |
| A1679 | C1401 | U1482 | A1401 | G1294 | G1208 | G1126 | G1058 | C979  | C905 | U824 | U719 | A532 | A432 | A432 |
| A1680 | C1402 | U1483 | A1402 | G1295 | G1209 | G1127 | G1059 | C980  | C906 | U825 | U720 | A532 | A432 | A432 |
| A1681 | C1403 | U1484 | A1403 | G1296 | G1210 | G1128 | G1060 | C981  | C907 | U826 | U721 | A532 | A432 | A432 |
| A1682 | C1404 | U1485 | A1404 | G1297 | G1211 | G1129 | G1061 | C982  | C908 | U827 | U722 | A532 | A432 | A432 |
| A1683 | C1405 | U1486 | A1405 | G1298 | G1212 | G1130 | U1062 | C983  | C909 | U828 | U723 | A532 | A432 | A432 |
| A1684 | C1406 | U1487 | A1406 | G1299 | G1213 | G1131 | C1063 | C984  | C910 | U829 | U724 | A532 | A432 | A432 |
| A1685 | C1407 | U1488 | A1407 | G1300 | G1214 | G1132 | U1064 | C985  | C911 | U830 | U725 | A532 | A432 | A432 |
| A1686 | C1408 | U1489 | A1408 | G1301 | A1214 | G1133 | U1065 | C986  | C912 | U831 | U726 | A532 | A432 | A432 |
| A1687 | C1409 | U1490 | A1409 | G1302 | G1215 | G1134 | U1066 | C987  | C913 | U832 | U727 | A532 | A432 | A432 |
| A1688 | C1410 | U1491 | A1410 | G1303 | G1216 | G1135 | U1067 | C988  | C914 | U833 | U728 | A532 | A432 | A432 |
| A1689 | C1411 | U1492 | A1411 | G1304 | G1217 | G1136 | U1068 | C989  | C915 | U834 | U729 | A532 | A432 | A432 |
| A1690 | C1412 | U1493 | A1412 | G1305 | G1218 | G1137 | U1069 | C990  | C916 | U835 | U730 | A532 | A432 | A432 |
| A1691 | C1413 | U1494 | A1413 | G1306 | G1219 | G1138 | U1070 | C991  | C917 | U836 | U731 | A532 | A432 | A432 |
| A1692 | C1414 | U1495 | A1414 | G1307 | G1220 | G1139 | U1071 | C992  | C918 | U837 | U732 | A532 | A432 | A432 |
| A1693 | C1415 | U1496 | A1415 | G1308 | G1221 | G1140 | U1072 | C993  | C919 | U838 | U733 | A532 | A432 | A432 |
| A1694 | C1416 | U1497 | A1416 | G1309 | G1222 | G1141 | U1073 | C994  | C920 | U839 | U734 | A532 | A432 | A432 |
| A1695 | C1417 | U1498 | A1417 | G1310 | G1223 | G1142 | U1074 | C995  | C921 | U840 | U735 | A532 | A432 | A432 |
| A1696 | C1418 | U1499 | A1418 | G1311 | G1224 | G1143 | U1075 | C996  | C922 | U841 | U736 | A532 | A432 | A432 |
| A1697 | C1419 | U1500 | A1419 | G1312 | G1225 | G1144 | U1076 | C997  | C923 | U842 | U737 | A532 | A432 | A432 |
| A1698 | C1420 | U1501 | A1420 | G1313 | G1226 | G1145 | U1077 | C998  | C924 | U843 | U738 | A532 | A432 | A432 |
| A1699 | C1421 | U1502 | A1421 | G1314 | G1227 | G1146 | U1078 | C999  | C925 | U844 | U739 | A532 | A432 | A432 |
| A1700 | C1422 | U1503 | A1422 | G1315 | G1228 | G1147 | U1079 | C1000 | C926 | U845 | U740 | A532 | A432 | A432 |
| A1701 | C1423 | U1504 | A1423 | G1316 | G1229 | G1148 | U1080 | C1001 | C927 | U846 | U741 | A532 | A432 | A432 |
| A1702 | C1424 | U1505 | A1424 | G1317 | G1230 | G1149 | U1081 | C1002 | C928 | U847 | U742 | A532 | A432 | A432 |
| A1703 | C1425 | U1506 | A1425 | G1318 | G1231 | G1150 | U1082 | C1003 | C929 | U848 | U743 | A532 | A432 | A432 |
| A1704 | C1426 | U1507 | A1426 | G1319 | G1232 | G1151 | U1083 | C1004 | C930 | U849 | U744 | A532 | A432 | A432 |
| A1705 | C1427 | U1508 | A1427 | G1320 | G1233 | G1152 | U1084 | C1005 | C931 | U850 | U745 | A532 | A432 | A432 |
| A1706 | C1428 | U1509 | A1428 | G1321 | G1234 | G1153 | U1085 | C1006 | C932 | U851 | U746 | A532 | A432 | A432 |
| A1707 | C1429 | U1510 | A1429 | G1322 | G1235 | G1154 | U1086 | C1007 | C933 | U852 | U747 | A532 | A432 | A432 |
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| A1709 | C1431 | U1512 | A1431 | G1324 | G1237 | G1156 | U1088 | C1009 | C935 | U854 | U749 | A532 | A432 | A432 |
| A1710 | C1432 | U1513 | A1432 | G1325 | G1238 | G1157 | U1089 | C1010 | C936 | U855 | U750 | A532 | A432 | A432 |
| A1711 | C1433 | U1514 | A1433 | G1326 | G1239 | G1158 | U1090 | C1011 | C937 | U856 | U751 | A532 | A432 | A432 |
| A1712 | C1434 | U1515 | A1434 | G1327 | G1240 | G1159 | U1091 | C1012 | C938 | U857 | U752 | A532 | A432 | A432 |
| A1713 | C1435 | U1516 | A1435 | G1328 | G1241 | G1160 | U1092 | C1013 | C939 | U858 | U753 | A532 | A432 | A432 |
| A1714 | C1436 | U1517 | A1436 | G1329 | G1242 | G1161 | U1093 | C1014 | C940 | U859 | U754 | A532 | A432 | A432 |
| A1715 | C1437 | U1518 | A1437 | G1330 | G1243 | G1162 | U1094 | C1015 | C941 | U860 | U755 | A532 | A432 | A432 |
| A1716 | C1438 | U1519 | A1438 | G1331 | G1244 | G1163 | U1095 | C1016 | C942 | U861 | U756 | A532 | A432 | A432 |
| A1717 | C1439 | U1520 | A1439 | G1332 | G1245 | G1164 | U1096 | C1017 | C943 | U862 | U757 | A532 | A432 | A432 |
| A1718 | C1440 | U1521 | A1440 | G1333 | G1246 | G1165 | U1097 | C1018 | C944 | U863 | U758 | A532 | A432 | A432 |
| A1719 | C1441 | U1522 | A1441 | G1334 | G1247 | G1166 | U1098 | C1019 | C945 | U864 | U759 | A532 | A432 | A432 |
| A1720 | C1442 | U1523 | A1442 | G1335 | G1248 | G1167 | U1099 | C1020 | C946 | U865 | U760 | A532 | A432 | A432 |
| A1721 | C1443 | U1524 | A1443 | G1336 | G1249 | G1168 | U1100 | C1021 | C947 | U866 | U761 | A532 | A432 | A432 |
| A1722 | C1444 | U1525 | A1444 | G1337 | G1250 | G1169 | U1101 | C1022 | C948 | U867 | U762 | A532 | A432 | A432 |
| A1723 | C1445 | U1526 | A1445 | G1338 | G1251 | G1170 | U1102 | C1023 | C949 | U868 | U763 | A532 | A432 | A432 |
| A1724 | C1446 | U1527 | A1446 | G1339 | G1252 | G1171 | U1103 | C1024 | C950 | U869 | U764 | A532 | A432 | A432 |
| A1725 | C1447 | U1528 | A1447 | G1340 | G1253 | G1172 | U1104 | C1025 | C951 | U870 | U765 | A532 | A432 | A432 |
| A1726 | C1448 | U1529 | A1448 | G1341 | G1254 | G1173 | U1105 | C1026 | C952 | U871 | U766 | A532 | A432 | A432 |
| A1727 | C1449 | U1530 | A1449 | G1342 | G1255 | G1174 | U1106 | C1027 | C953 | U872 | U767 | A532 | A432 | A432 |
| A1728 | C1450 | U1531 | A1450 | G1343 | G1256 | G1175 | U1107 | C1028 | C954 | U873 | U768 | A532 | A432 | A432 |
| A1729 | C1451 | U1532 | A1451 | G1344 | G1257 | G1176 | U1108 | C1029 | C955 | U874 | U769 | A532 | A432 | A432 |
| A1730 | C1452 | U1533 | A1452 | G1345 | G1258 | G1177 | U1109 | C1030 | C956 | U875 | U770 | A532 | A432 | A432 |
| A1731 | C1453 | U1534 | A1453 | G1346 | G1259 | G1178 | U1110 | C1031 | C957 | U876 | U771 | A532 | A432 | A432 |
| A1732 | C1454 | U1535 | A1454 | G1347 | G1260 | G1179 | U1111 | C1032 | C958 | U877 | U772 | A532 | A432 | A432 |
| A1733 | C1455 | U1536 | A1455 | G1348 | G1261 | G1180 | U1112 | C1033 | C959 | U878 | U773 | A532 | A432 | A432 |
| A1734 | C1456 | U1537 | A14   |       |       |       |       |       |      |      |      |      |      |      |

|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G2862 | G2789 | G2708 | G2612 | G2529 | G2373 | G2458 | G2459 | G2529 | A2212 | G2133 | C2055 | U1982 | G1907 | G1823 | U1729 |
| G2867 | U2790 | G2709 | U2613 | A2530 | C2374 | A2459 | A2460 | A2530 | C2215 | A2134 | G2056 | G1983 | G1910 | G1824 | G1730 |
| A2873 | A2791 | G2710 | U2614 | G2531 | G2375 | A2461 | A2462 | G2532 | G2216 | U2139 | A2060 | A1987 | U     | G1825 | C1750 |
| C2874 | C2793 | G2711 | U2615 | G2533 | A2377 | C2462 | C2463 | G2534 | G2217 | G2140 | G2061 | G1991 | A1912 | U1826 | C1732 |
| C2880 | U2796 | G2712 | U2616 | G2535 | A2381 | G2464 | G2465 | G2536 | G2218 | G2141 | C2062 | G1992 | C1914 | G1828 | G1738 |
| A2883 | U2797 | G2713 | U2617 | U2537 | G2382 | C2466 | C2467 | G2538 | G2223 | C2146 | C2064 | U     | A1916 | A1746 | A1746 |
| U2884 | U2798 | G2714 | C2619 | C2538 | G2383 | C2468 | C2469 | G2539 | G2224 | A2147 | C2065 | C1996 | U     | G1830 | U1747 |
| G2885 | A2800 | U2719 | U2620 | A2542 | U2384 | A2476 | A2477 | G2543 | A2225 | U2148 | C2066 | C1997 | A1918 | C1832 | C1832 |
| U2891 | G2801 | G2720 | G2621 | G2544 | G2385 | A2478 | A2479 | U2545 | G2226 | U2149 | C2067 | C1998 | A1919 | U1834 | G1750 |
| C2902 | G2802 | G2721 | U2622 | A2547 | U2387 | G2480 | G2481 | U2548 | A2227 | C2150 | G     | U2075 | A1920 | G     | G1750 |
| G2903 | U2803 | C2722 | U2623 | U2548 | U2388 | U2470 | U2471 | U2549 | U2228 | A2154 | A2070 | C2000 | G1921 | G1763 | G1763 |
| U2904 | U2804 | C2723 | G2624 | G2549 | G2391 | U2472 | U2473 | G2550 | U2229 | G2157 | A2071 | C2001 | G1922 | A1754 | A1754 |
| C2905 | C2805 | A2725 | C2625 | G2550 | U2392 | U2474 | U2475 | G2551 | G2230 | C2158 | C2072 | G2002 | U1923 | A1755 | A1755 |
| U2906 | U2806 | A2726 | U2626 | C2551 | U2393 | C2476 | C2477 | U2552 | U2231 | G2159 | C2073 | C2006 | C1924 | G1840 | G1840 |
| U2907 | U2807 | A2727 | U2627 | U     | C2394 | A2478 | A2479 | U2553 | G2232 | G2160 | U     | U2007 | C1925 | U1841 | A1757 |
| G2908 | G2808 | U2728 | A2639 | G2554 | C2395 | U2477 | U2478 | U2554 | G2233 | C2161 | G2075 | G2007 | U1926 | G1842 | U1758 |
| A2809 | A2809 | U2728 | G2640 | U2554 | G2396 | A2478 | A2479 | U2555 | G2234 | G2162 | A2082 | G2010 | A1927 | C1843 | C1764 |
| A2810 | A2810 | G2731 | U2641 | U2555 | U2397 | U2479 | U2480 | U2556 | U2243 | C2163 | G2083 | U2011 | A1928 | C1844 | C1764 |
| G2811 | G2811 | G2732 | U2642 | G2556 | U2402 | U2481 | U2482 | G2557 | U2244 | A2164 | G2084 | U2012 | U1929 | G1845 | G1770 |
| A2812 | A2812 | U2740 | U2643 | C2558 | C2403 | A2483 | A2484 | G2558 | U2245 | C2165 | G2085 | G2013 | G1930 | G1846 | G1770 |
| A2813 | A2813 | A2741 | G2644 | U2559 | A2406 | G2485 | G2486 | U2559 | U2246 | G2166 | G2086 | A2014 | U1931 | A1847 | A1773 |
| C2815 | C2815 | G2742 | U2645 | G2560 | A2407 | G2487 | G2488 | U2560 | U2247 | G2167 | G2087 | A2015 | U1932 | A1848 | C1774 |
| G2816 | G2816 | U2743 | C2646 | G2561 | U2408 | U2489 | U2490 | U2561 | C2248 | A2169 | C2091 | U2016 | A1936 | A1853 | A1853 |
| U2817 | U2817 | G2744 | U2647 | U2562 | U2409 | U2491 | U2492 | U2562 | U2249 | A2170 | U2092 | U2017 | U1937 | A1854 | U1778 |
| G2818 | G2818 | A2745 | G2647 | U2563 | C2410 | U2493 | U2494 | U2563 | G2250 | A2171 | G2093 | G2020 | A1938 | U1855 | U1779 |
| G2819 | G2819 | A2746 | U2648 | U2564 | G2411 | U2495 | U2496 | U2564 | G2251 | A2172 | A2094 | A2020 | U     | U1856 | U1856 |
| A2820 | A2820 | A2747 | U2649 | U2565 | G2412 | U2497 | U2498 | U2565 | G2252 | U2173 | C2095 | C2021 | A1940 | G1857 | A1784 |
| C2821 | C2821 | U2748 | U2650 | U2566 | U2413 | U2499 | U2500 | U2566 | G2253 | C2175 | C2096 | U2022 | U1941 | A1785 | A1785 |
| G2822 | G2822 | U2749 | U2651 | U2567 | C2414 | U2501 | U2502 | U2567 | U2254 | A2176 | A2097 | G2023 | U1942 | A1786 | A1786 |
| A2823 | A2823 | C2755 | U2652 | G2568 | A2415 | U2503 | U2504 | U2568 | U2255 | C2177 | U2098 | C2024 | U1943 | G1862 | A1789 |
| C2824 | C2824 | U2756 | U2653 | U2569 | A2416 | U2505 | U2506 | U2569 | G2256 | C2178 | U2099 | C2025 | U1944 | G1945 | G1789 |
| G2825 | G2825 | A2757 | U2654 | U2570 | C2417 | U2507 | U2508 | U2570 | U2257 | C2179 | G2100 | U2026 | U1945 | C1790 | C1790 |
| U2833 | U2833 | A2758 | U2655 | G2571 | G2418 | U2509 | U2510 | U2571 | U2258 | U2180 | G2101 | G2027 | C1947 | A1791 | G1792 |
| G2834 | G2834 | G2759 | U2656 | U2572 | U2419 | U2511 | U2512 | U2572 | U2259 | U2181 | A2108 | U2028 | A1953 | G1869 | G1793 |
| A2835 | A2835 | U2760 | U2657 | U2573 | U2420 | U2513 | U2514 | U2573 | U2260 | U2182 | U2109 | G2029 | G1954 | C1870 | C1794 |
| G2838 | G2838 | A2761 | U2658 | U2574 | U2421 | U2515 | U2516 | U2574 | U2261 | A2183 | G2110 | A     | U1955 | A1871 | A1794 |
| C2839 | C2839 | C2762 | U2659 | U2575 | U2422 | U2517 | U2518 | U2575 | U2262 | U2184 | U2111 | G2031 | U1956 | C1795 | C1795 |
| C2840 | C2840 | U2763 | U2660 | U2576 | U2423 | U2519 | U2520 | U2576 | U2263 | U2185 | U2112 | G2032 | U1957 | A1872 | U1796 |
| C2841 | C2841 | U2764 | U2661 | U2577 | U2424 | U2521 | U2522 | U2577 | U2264 | U2186 | U2113 | U2033 | C1958 | G1873 | G1797 |
| U2845 | U2845 | U2765 | U2662 | U2578 | U2425 | U2523 | U2524 | U2578 | U2265 | U2187 | A2114 | U2034 | C1959 | C1874 | U1798 |
| G2846 | G2846 | A2766 | U2663 | U2579 | A2426 | U2525 | U2526 | U2579 | U2266 | U2188 | G2115 | G2035 | G1959 | G1799 | G1799 |
| U2847 | U2847 | C2767 | U2664 | U2580 | A2427 | U2527 | U2528 | U2580 | U2267 | U2189 | G2116 | C2036 | A1960 | C1800 | C1800 |
| G2848 | G2848 | U2768 | U2665 | U2581 | U2428 | U2529 | U2530 | U2581 | U2268 | U2190 | G2117 | A2037 | C1961 | A1801 | A1801 |
| U2849 | U2849 | U2769 | U2666 | U2582 | U2429 | U2531 | U2532 | U2582 | U2269 | U2191 | A2117 | G2038 | C     | A1802 | A1802 |
| A2850 | A2850 | U2770 | U2667 | U2583 | U2430 | U2533 | U2534 | U2583 | U2270 | U2192 | G2118 | U2039 | U1963 | A1881 | A1881 |
| G2851 | G2851 | G2771 | U2668 | U2584 | U2431 | U2535 | U2536 | U2584 | U2271 | U2193 | U2119 | G2040 | C1965 | U1882 | U1882 |
| C2852 | C2852 | U2772 | U2669 | U2585 | U2432 | U2537 | U2538 | U2585 | U2272 | U2194 | G2120 | U2041 | C1966 | U1883 | A1808 |
| U2856 | U2856 | U2773 | U2670 | U2586 | U2433 | U2539 | U2540 | U2586 | U2273 | U2195 | G2121 | U2042 | C1967 | G1884 | A1808 |
| G2859 | G2859 | U2774 | U2671 | U2587 | U2434 | U2541 | U2542 | U2587 | U2274 | U2196 | G2122 | U2043 | U1970 | A1889 | A1889 |
| A2860 | A2860 | C2785 | U2672 | U2588 | U2435 | U2543 | U2544 | U2588 | U2275 | U2197 | G2123 | U2044 | A1971 | A1890 | G1816 |
| U2861 | U2861 | U2788 | U2673 | U2589 | U2436 | U2545 | U2546 | U2589 | U2276 | U2198 | G2124 | G2045 | A1972 | U1817 | G1817 |
|       |       |       | U2674 | U2590 | U2437 | U2547 | U2548 | U2590 | U2277 | A2199 | G2125 | G2046 | G1973 | U1818 | U1818 |
|       |       |       | U2675 | U2591 | U2438 | U2549 | U2550 | U2591 | U2278 | U2200 | G2126 | G2047 | A1974 | U1819 | A1819 |
|       |       |       | U2676 | U2592 | U2439 | U2551 | U2552 | U2592 | U2279 | G2204 | G2127 | G2048 | A1975 | U1820 | U1820 |
|       |       |       | U2677 | U2593 | U2440 | U2553 | U2554 | U2593 | U2280 | A2205 | G2128 | G2049 | A1976 | A1900 | A1900 |
|       |       |       | U2678 | U2594 | U2441 | U2555 | U2556 | U2594 | U2281 | C2206 | G2129 | G2050 | A1977 | G1972 | G1972 |
|       |       |       | U2679 | U2595 | U2442 | U2557 | U2558 | U2595 | U2282 | U2207 | G2130 | A2051 | A1978 | U1971 | G1971 |
|       |       |       | U2680 | U2596 | U2443 | U2559 | U2560 | U2596 | U2283 | A2211 | U2131 | A2052 | A1979 | G1980 | G1980 |
|       |       |       | U2681 | U2597 | U2444 | U2561 | U2562 | U2597 | U2284 |       | U2132 |       | A1980 | G1906 | G1906 |
|       |       |       | U2682 | U2598 | U2445 | U2563 | U2564 | U2598 | U2285 |       |       |       |       |       |       |
|       |       |       | U2683 | U2599 | U2446 | U2565 | U2566 | U2599 | U2286 |       |       |       |       |       |       |
|       |       |       | U2684 | U2600 | U2447 | U2567 | U2568 | U2600 | U2287 |       |       |       |       |       |       |
|       |       |       | U2685 | U2601 | U2448 | U2569 | U2570 | U2601 | U2288 |       |       |       |       |       |       |
|       |       |       | U2686 | U2602 | U2449 | U2571 | U2572 | U2602 | U2289 |       |       |       |       |       |       |
|       |       |       | U2687 | U2603 | U2450 | U2573 | U2574 | U2603 | U2290 |       |       |       |       |       |       |
|       |       |       | U2688 | U2604 | U2451 | U2575 | U2576 | U2604 | U2291 |       |       |       |       |       |       |
|       |       |       | U2689 | U2605 | U2452 | U2577 | U2578 | U2605 | U2292 |       |       |       |       |       |       |
|       |       |       | U2690 | U2606 | U2453 | U2579 | U2580 | U2606 | U2293 |       |       |       |       |       |       |
|       |       |       | U2691 | U2607 | U2454 | U2581 | U2582 | U2607 | U2294 |       |       |       |       |       |       |
|       |       |       | U2692 | U2608 | U2455 | U2583 | U2584 | U2608 | U2295 |       |       |       |       |       |       |
|       |       |       | U2693 | U2609 | U2456 | U2585 | U2586 | U2609 | U2296 |       |       |       |       |       |       |
|       |       |       | U2694 | U2610 | U2457 | U2587 | U2588 | U2610 | U2297 |       |       |       |       |       |       |
|       |       |       | U2695 | U2611 | U2458 | U2589 | U2590 | U2611 | U2298 |       |       |       |       |       |       |
|       |       |       | U2696 | U2612 | U2459 | U2591 | U2592 | U2612 | U2299 |       |       |       |       |       |       |
|       |       |       | U2697 | U2613 | U2460 | U2593 | U2594 | U2613 | U2300 |       |       |       |       |       |       |
|       |       |       | U2698 | U2614 | U2461 | U2595 | U2596 | U2614 | U2301 |       |       |       |       |       |       |
|       |       |       | U2699 | U2615 | U2462 | U2597 | U2598 | U2615 | U2302 |       |       |       |       |       |       |
|       |       |       | U2700 | U2616 | U2463 | U2599 | U2600 | U2616 | U2303 |       |       |       |       |       |       |
|       |       |       | U2701 | U2617 | U2464 | U2601 | U2602 | U2617 | U2304 |       |       |       |       |       |       |
|       |       |       | U2702 | U2618 | U2465 | U2603 | U2604 | U2618 | U2305 |       |       |       |       |       |       |
|       |       |       | U2703 | U2619 | U2466 | U2605 | U2606 | U2619 | U2306 |       |       |       |       |       |       |
|       |       |       | U2704 | U2620 | U2467 | U2607 | U2608 | U2620 | U2307 |       |       |       |       |       |       |
|       |       |       | U2705 | U2621 | U2468 | U2609 | U2610 | U2621 | U2308 |       |       |       |       |       |       |
|       |       |       | U2706 | U2622 | U2469 | U2611 | U2612 | U2622 | U2309 |       |       |       |       |       |       |
|       |       |       | U2707 | U2623 | U2470 | U2613 | U2614 | U2623 | U2310 |       |       |       |       |       |       |
|       |       |       | U2708 | U2624 | U2471 | U2615 | U2616 | U2624 | U2311 |       |       |       |       |       |       |
|       |       |       | U2709 | U2625 | U2472 | U2617 | U2618 | U2625 | U2312 |       |       |       |       |       |       |
|       |       |       | U2710 | U2626 | U2473 | U2619 | U2620 | U2626 | U2313 |       |       |       |       |       |       |
|       |       |       | U2711 | U2627 | U2474 | U2621 | U262  |       |       |       |       |       |       |       |       |

- Molecule 41: 50S ribosomal protein L27

Chain b: 



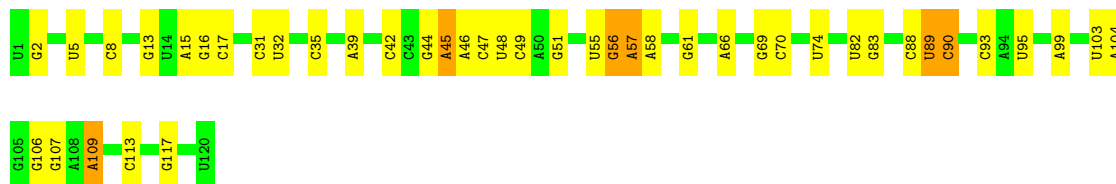
- Molecule 42: 50S ribosomal protein L28

Chain c: 



- Molecule 43: 5S rRNA

Chain d: 



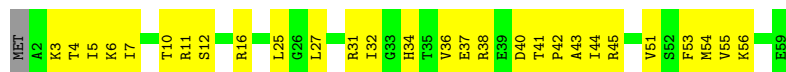
- Molecule 44: 50S ribosomal protein L29

Chain e: 



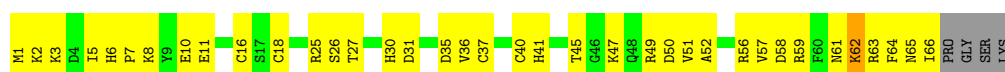
- Molecule 45: 50S ribosomal protein L30

Chain f: 



- Molecule 46: 50S ribosomal protein L31

Chain g: 



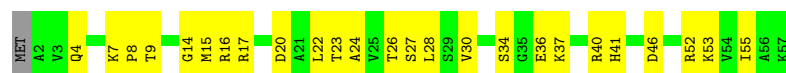
- Molecule 47: 50S ribosomal protein L2

Chain h: 



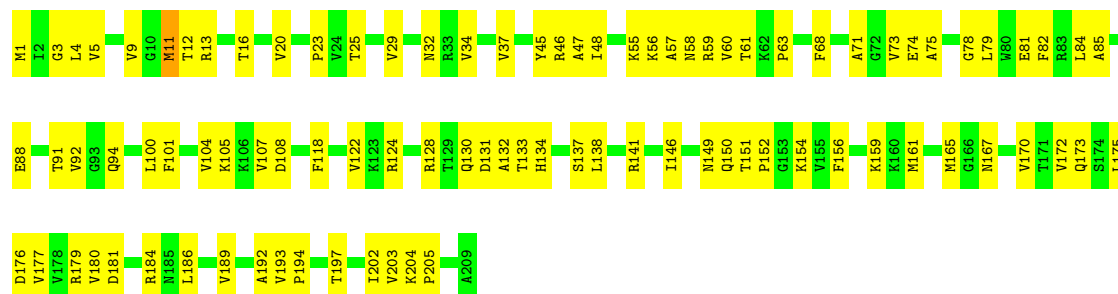
• Molecule 48: 50S ribosomal protein L32

Chain i: 54% 44%



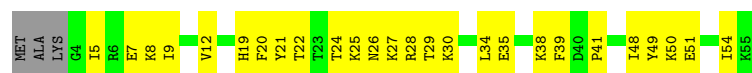
• Molecule 49: 50S ribosomal protein L3

Chain j: 56% 44%



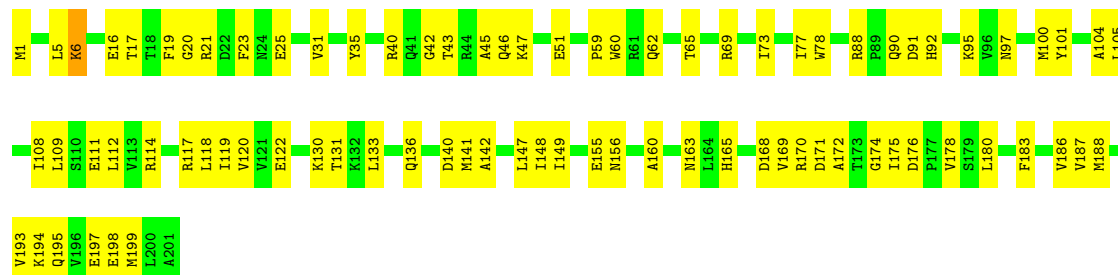
• Molecule 50: 50S ribosomal protein L33

Chain k: 47% 47% 5%



• Molecule 51: 50S ribosomal protein L4

Chain l: 59% 40%

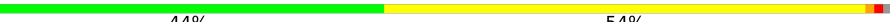


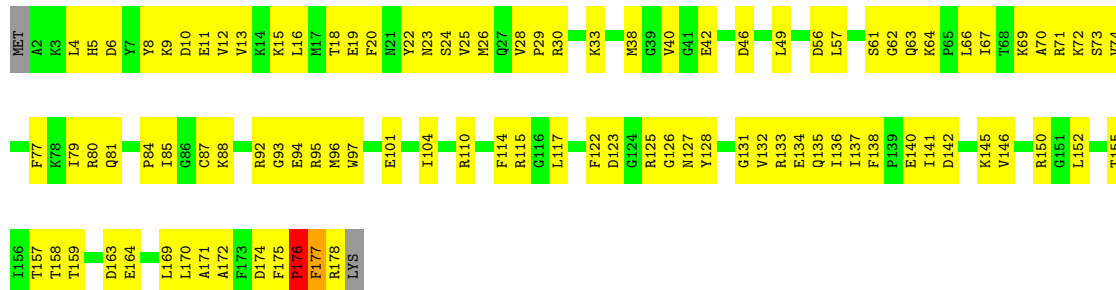
- Molecule 52: 50S ribosomal protein L34

Chain m:  57% 43%



- Molecule 53: 50S ribosomal protein L5

Chain n:  44% 54% ...



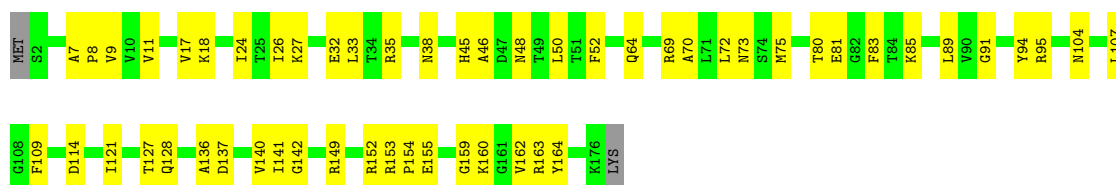
- Molecule 54: 50S ribosomal protein L35

Chain o:  58% 35% 5%



- Molecule 55: 50S ribosomal protein L6

Chain p:  68% 31%



- Molecule 56: 50S ribosomal protein L36

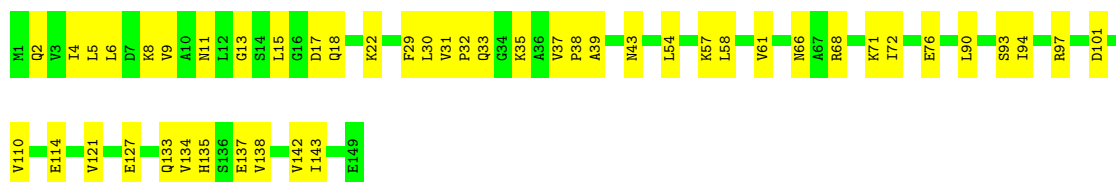
Chain q:  61% 39%



- Molecule 57: 50S ribosomal protein L9

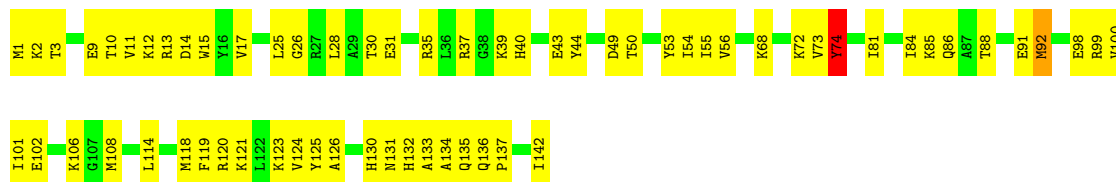
Chain r:  68% 32%





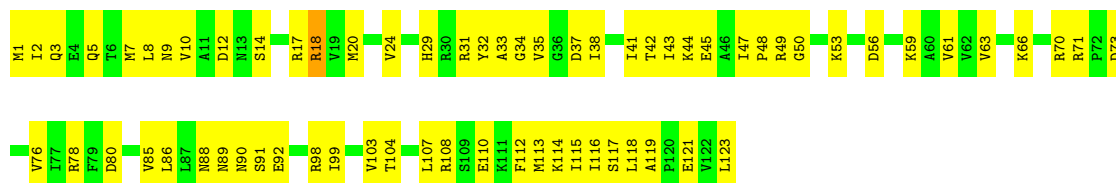
• Molecule 58: 50S ribosomal protein L13

Chain s: 55% 44% ..



• Molecule 59: 50S ribosomal protein L14

Chain t: 46% 54% .



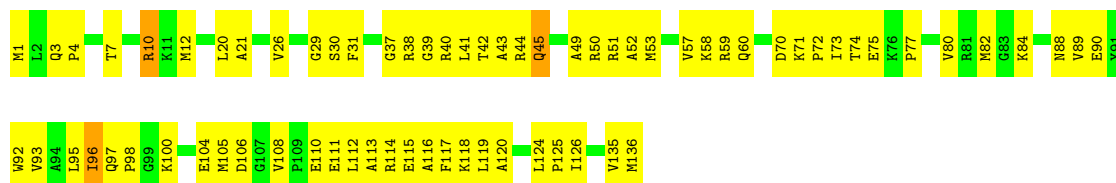
• Molecule 60: 50S ribosomal protein L15

Chain u: 62% 37% .



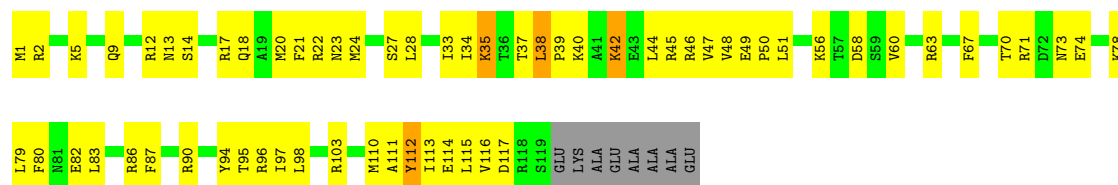
• Molecule 61: 50S ribosomal protein L16

Chain v: 49% 49% .



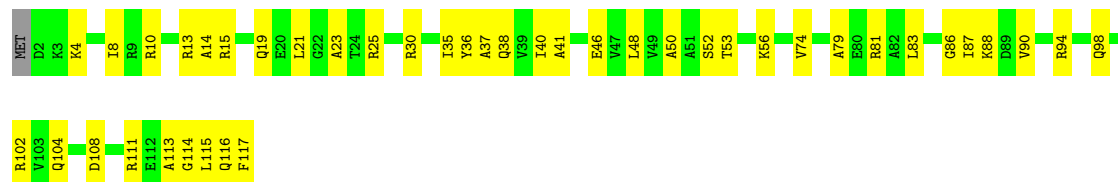
• Molecule 62: 50S ribosomal protein L17

Chain w: 44% 46% 6% .



• Molecule 63: 50S ribosomal protein L18

Chain x: 63% 36%



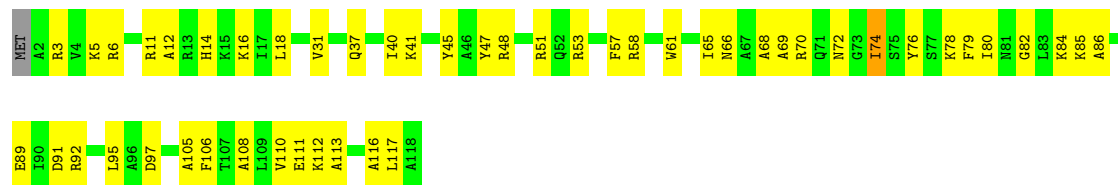
• Molecule 64: 50S ribosomal protein L19

Chain y: 63% 37%



• Molecule 65: 50S ribosomal protein L20

Chain z: 58% 41%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 10509                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TALOS ARCTICA                       | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 28                                      | Depositor |
| Minimum defocus (nm)                 | 1250                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.032                                   | Depositor |
| Minimum map value                    | -0.007                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.002                                   | Depositor |
| Recommended contour level            | 0.0025                                  | Depositor |
| Map size (Å)                         | 531.968, 531.968, 531.968               | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.039, 1.039, 1.039                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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   | 0     | 0.43         | 0/829         | 0.51        | 0/1107         |
| 2   | 1     | 0.60         | 0/864         | 0.63        | 0/1156         |
| 3   | 2     | 0.55         | 1/752 (0.1%)  | 0.67        | 0/1005         |
| 4   | 3     | 0.35         | 0/796         | 0.49        | 0/1062         |
| 5   | 4     | 0.57         | 0/766         | 0.63        | 0/1025         |
| 6   | 5     | 0.56         | 0/816         | 0.77        | 0/1259         |
| 7   | 6     | 0.56         | 0/783         | 0.77        | 0/1203         |
| 8   | 7     | 0.56         | 2/879 (0.2%)  | 0.86        | 3/1364 (0.2%)  |
| 9   | 9     | 0.36         | 0/1131        | 0.74        | 2/1524 (0.1%)  |
| 10  | A     | 0.27         | 0/1810        | 0.58        | 0/2821         |
| 10  | B     | 0.27         | 0/1810        | 0.58        | 0/2821         |
| 11  | AA    | 0.38         | 0/10547       | 0.62        | 0/14232        |
| 12  | AB    | 0.46         | 0/1317        | 1.10        | 9/1786 (0.5%)  |
| 13  | AC    | 0.38         | 0/1718        | 0.61        | 0/2328         |
| 13  | AD    | 0.32         | 0/1696        | 0.60        | 0/2298         |
| 14  | AE    | 0.39         | 0/10561       | 0.64        | 5/14258 (0.0%) |
| 15  | AF    | 0.29         | 0/652         | 0.61        | 0/879          |
| 16  | C     | 0.67         | 0/553         | 0.81        | 1/743 (0.1%)   |
| 17  | D     | 0.29         | 0/36610       | 0.41        | 9/57091 (0.0%) |
| 18  | E     | 0.61         | 0/675         | 0.72        | 0/895          |
| 19  | F     | 0.53         | 0/597         | 0.60        | 0/792          |
| 20  | G     | 0.68         | 5/1791 (0.3%) | 0.79        | 8/2413 (0.3%)  |
| 21  | H     | 0.38         | 0/1746        | 0.81        | 0/2382         |
| 22  | I     | 0.57         | 1/1663 (0.1%) | 0.68        | 4/2241 (0.2%)  |
| 23  | J     | 0.46         | 0/1665        | 0.58        | 0/2227         |
| 24  | K     | 0.72         | 2/1165 (0.2%) | 0.86        | 6/1568 (0.4%)  |
| 25  | L     | 0.68         | 1/867 (0.1%)  | 0.79        | 1/1171 (0.1%)  |
| 26  | M     | 0.56         | 0/1195        | 0.69        | 2/1602 (0.1%)  |
| 27  | N     | 0.50         | 0/989         | 0.58        | 0/1326         |
| 28  | O     | 0.66         | 3/1034 (0.3%) | 0.79        | 3/1375 (0.2%)  |
| 29  | P     | 0.49         | 0/800         | 0.65        | 1/1082 (0.1%)  |
| 30  | Q     | 0.72         | 2/893 (0.2%)  | 0.76        | 2/1205 (0.2%)  |

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5          |
| 31  | R     | 0.49         | 0/952            | 0.59        | 0/1274           |
| 32  | S     | 0.53         | 0/817            | 0.61        | 0/1088           |
| 33  | T     | 0.57         | 1/722 (0.1%)     | 0.68        | 0/964            |
| 34  | U     | 0.41         | 0/659            | 0.53        | 0/884            |
| 35  | V     | 0.49         | 0/657            | 0.63        | 0/881            |
| 36  | W     | 0.56         | 1/680 (0.1%)     | 0.62        | 1/915 (0.1%)     |
| 37  | X     | 0.45         | 0/909            | 0.72        | 1/1215 (0.1%)    |
| 38  | Y     | 0.38         | 2/1046 (0.2%)    | 0.66        | 2/1410 (0.1%)    |
| 39  | Z     | 0.13         | 0/227            | 0.41        | 0/304            |
| 40  | a     | 0.30         | 0/69247          | 0.43        | 10/107985 (0.0%) |
| 41  | b     | 0.42         | 0/589            | 0.56        | 0/779            |
| 42  | c     | 0.51         | 0/635            | 0.61        | 0/848            |
| 43  | d     | 0.25         | 0/2872           | 0.37        | 0/4478           |
| 44  | e     | 0.69         | 2/502 (0.4%)     | 0.65        | 1/667 (0.1%)     |
| 45  | f     | 0.52         | 0/452            | 0.57        | 0/605            |
| 46  | g     | 0.45         | 1/531 (0.2%)     | 0.64        | 0/709            |
| 47  | h     | 0.49         | 1/2121 (0.0%)    | 0.58        | 1/2852 (0.0%)    |
| 48  | i     | 0.41         | 0/450            | 0.55        | 0/599            |
| 49  | j     | 0.51         | 0/1586           | 0.57        | 1/2134 (0.0%)    |
| 50  | k     | 0.45         | 0/433            | 0.62        | 0/576            |
| 51  | l     | 0.51         | 1/1571 (0.1%)    | 0.62        | 0/2113           |
| 52  | m     | 0.45         | 0/380            | 0.56        | 0/498            |
| 53  | n     | 0.46         | 0/1434           | 0.66        | 1/1926 (0.1%)    |
| 54  | o     | 0.51         | 0/513            | 0.71        | 1/676 (0.1%)     |
| 55  | p     | 0.41         | 0/1333           | 0.62        | 2/1805 (0.1%)    |
| 56  | q     | 0.46         | 0/303            | 0.64        | 0/397            |
| 57  | r     | 0.28         | 0/1122           | 0.48        | 0/1515           |
| 58  | s     | 0.70         | 2/1152 (0.2%)    | 0.74        | 2/1551 (0.1%)    |
| 59  | t     | 0.52         | 0/955            | 0.75        | 3/1279 (0.2%)    |
| 60  | u     | 0.43         | 0/1062           | 0.59        | 0/1413           |
| 61  | v     | 0.60         | 1/1093 (0.1%)    | 0.77        | 3/1460 (0.2%)    |
| 62  | w     | 0.83         | 3/964 (0.3%)     | 0.80        | 3/1289 (0.2%)    |
| 63  | x     | 0.34         | 0/902            | 0.50        | 0/1209           |
| 64  | y     | 0.41         | 0/929            | 0.54        | 0/1242           |
| 65  | z     | 0.61         | 2/960 (0.2%)     | 0.62        | 0/1278           |
| All | All   | 0.39         | 34/190730 (0.0%) | 0.53        | 88/281059 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 9   | 9     | 0                   | 3                   |
| 12  | AB    | 0                   | 10                  |
| 13  | AC    | 0                   | 1                   |
| 13  | AD    | 0                   | 1                   |
| 14  | AE    | 0                   | 4                   |
| 20  | G     | 0                   | 1                   |
| 21  | H     | 0                   | 5                   |
| 22  | I     | 0                   | 1                   |
| 24  | K     | 0                   | 2                   |
| 28  | O     | 0                   | 1                   |
| 37  | X     | 0                   | 1                   |
| 38  | Y     | 0                   | 1                   |
| 53  | n     | 0                   | 1                   |
| 54  | o     | 0                   | 1                   |
| 58  | s     | 0                   | 1                   |
| 60  | u     | 0                   | 2                   |
| All | All   | 0                   | 36                  |

All (34) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 62  | w     | 35  | LYS  | CE-NZ   | -12.77 | 1.11        | 1.49     |
| 28  | O     | 80  | ARG  | CD-NE   | -10.47 | 1.31        | 1.46     |
| 62  | w     | 42  | LYS  | CD-CE   | -9.38  | 1.24        | 1.52     |
| 24  | K     | 45  | ARG  | CG-CD   | 7.74   | 1.75        | 1.52     |
| 65  | z     | 74  | ILE  | CG1-CD1 | 7.59   | 1.81        | 1.51     |
| 8   | 7     | 37  | G    | C1'-N9  | -7.57  | 1.36        | 1.48     |
| 20  | G     | 19  | GLN  | CB-CG   | -7.56  | 1.29        | 1.52     |
| 28  | O     | 118 | LEU  | CG-CD2  | -7.31  | 1.28        | 1.52     |
| 36  | W     | 66  | MET  | CG-SD   | -7.21  | 1.62        | 1.80     |
| 25  | L     | 42  | TRP  | CB-CG   | -7.19  | 1.27        | 1.50     |
| 44  | e     | 46  | VAL  | CB-CG1  | -7.11  | 1.29        | 1.52     |
| 58  | s     | 74  | TYR  | CZ-OH   | -7.11  | 1.23        | 1.38     |
| 8   | 7     | 2   | U    | C1'-N1  | 7.07   | 1.59        | 1.48     |
| 3   | 2     | 5   | GLU  | CG-CD   | -6.96  | 1.34        | 1.52     |
| 30  | Q     | 106 | ARG  | CD-NE   | -6.40  | 1.37        | 1.46     |
| 28  | O     | 80  | ARG  | CZ-NH2  | 6.33   | 1.41        | 1.33     |
| 20  | G     | 158 | PRO  | CA-C    | -6.18  | 1.44        | 1.52     |
| 47  | h     | 181 | MET  | CG-SD   | -6.05  | 1.65        | 1.80     |
| 20  | G     | 158 | PRO  | CG-CD   | 6.03   | 1.71        | 1.50     |
| 38  | Y     | 5   | GLN  | CB-CG   | -6.01  | 1.34        | 1.52     |
| 65  | z     | 74  | ILE  | CB-CG2  | -6.00  | 1.32        | 1.52     |
| 58  | s     | 92  | MET  | CG-SD   | -5.95  | 1.65        | 1.80     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 24  | K     | 45  | ARG  | CD-NE  | 5.85  | 1.54        | 1.46     |
| 51  | l     | 6   | LYS  | CE-NZ  | -5.81 | 1.31        | 1.49     |
| 20  | G     | 157 | LEU  | C-O    | -5.79 | 1.15        | 1.24     |
| 33  | T     | 3   | LEU  | CG-CD2 | -5.63 | 1.33        | 1.52     |
| 46  | g     | 62  | LYS  | CE-NZ  | -5.53 | 1.32        | 1.49     |
| 38  | Y     | 5   | GLN  | CA-C   | -5.51 | 1.45        | 1.52     |
| 44  | e     | 25  | GLN  | CB-CG  | -5.33 | 1.36        | 1.52     |
| 22  | I     | 134 | MET  | CB-CG  | -5.26 | 1.36        | 1.52     |
| 20  | G     | 19  | GLN  | CD-NE2 | -5.16 | 1.22        | 1.33     |
| 30  | Q     | 119 | ASN  | CG-ND2 | 5.16  | 1.44        | 1.33     |
| 61  | v     | 45  | GLN  | CB-CG  | -5.10 | 1.37        | 1.52     |
| 62  | w     | 38  | LEU  | N-CA   | -5.00 | 1.42        | 1.46     |

All (88) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 24  | K     | 71   | MET  | CG-SD-CE    | -11.34 | 75.95       | 100.90   |
| 20  | G     | 158  | PRO  | N-CD-CG     | -10.97 | 86.74       | 103.20   |
| 12  | AB    | 141  | LEU  | CA-C-N      | -10.59 | 106.28      | 122.16   |
| 12  | AB    | 141  | LEU  | C-N-CA      | -10.59 | 106.28      | 122.16   |
| 25  | L     | 102  | MET  | CA-CB-CG    | -9.59  | 94.91       | 114.10   |
| 58  | s     | 92   | MET  | CG-SD-CE    | -9.36  | 80.31       | 100.90   |
| 20  | G     | 113  | ARG  | NE-CZ-NH2   | 9.18   | 127.46      | 119.20   |
| 8   | 7     | 1    | A    | O3'-P-O5'   | -8.64  | 91.04       | 104.00   |
| 24  | K     | 78   | ASN  | N-CA-CB     | -8.53  | 96.08       | 110.49   |
| 8   | 7     | 4    | U    | C2'-C3'-O3' | 8.23   | 121.84      | 109.50   |
| 59  | t     | 18   | ARG  | NE-CZ-NH2   | 8.08   | 126.47      | 119.20   |
| 54  | o     | 30   | ARG  | NE-CZ-NH1   | -7.65  | 113.85      | 121.50   |
| 16  | C     | 73   | ARG  | NE-CZ-NH2   | 7.49   | 125.94      | 119.20   |
| 28  | O     | 80   | ARG  | CG-CD-NE    | 7.40   | 128.27      | 112.00   |
| 62  | w     | 112  | TYR  | CZ-CE2-CD2  | -7.35  | 106.37      | 119.60   |
| 22  | I     | 134  | MET  | CB-CG-SD    | -7.18  | 91.15       | 112.70   |
| 20  | G     | 158  | PRO  | CA-N-CD     | -7.07  | 102.10      | 112.00   |
| 61  | v     | 96   | ILE  | CA-C-N      | 7.07   | 132.34      | 121.03   |
| 61  | v     | 96   | ILE  | C-N-CA      | 7.07   | 132.34      | 121.03   |
| 20  | G     | 19   | GLN  | CA-CB-CG    | 7.01   | 128.13      | 114.10   |
| 59  | t     | 18   | ARG  | NE-CZ-NH1   | -7.01  | 114.49      | 121.50   |
| 28  | O     | 80   | ARG  | CB-CG-CD    | -6.94  | 95.33       | 111.30   |
| 40  | a     | 2334 | U    | OP2-P-O3'   | -6.94  | 87.17       | 108.00   |
| 17  | D     | 37   | U    | N3-C4-O4    | -6.63  | 99.52       | 119.40   |
| 62  | w     | 112  | TYR  | OH-CZ-CE2   | -6.57  | 100.19      | 119.90   |
| 17  | D     | 718  | A    | P-O5'-C5'   | -6.56  | 111.06      | 120.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 30  | Q     | 110  | ILE  | N-CA-C     | -6.48 | 99.04       | 108.11   |
| 17  | D     | 827  | U    | N3-C4-O4   | -6.41 | 100.17      | 119.40   |
| 40  | a     | 1019 | U    | N3-C4-O4   | -6.37 | 100.30      | 119.40   |
| 17  | D     | 1358 | U    | N3-C4-O4   | -6.33 | 100.42      | 119.40   |
| 58  | s     | 92   | MET  | CB-CG-SD   | -6.32 | 93.75       | 112.70   |
| 36  | W     | 40   | ILE  | CA-CB-CG1  | -6.31 | 99.67       | 110.40   |
| 12  | AB    | 99   | TYR  | CA-C-N     | 6.29  | 137.14      | 121.80   |
| 12  | AB    | 99   | TYR  | C-N-CA     | 6.29  | 137.14      | 121.80   |
| 40  | a     | 1019 | U    | C5-C4-O4   | 6.14  | 144.33      | 125.90   |
| 28  | O     | 103  | PHE  | CD1-CE1-CZ | -6.00 | 109.20      | 120.00   |
| 40  | a     | 1082 | U    | N3-C4-O4   | -5.94 | 101.58      | 119.40   |
| 40  | a     | 2613 | U    | N3-C4-O4   | -5.92 | 101.64      | 119.40   |
| 40  | a     | 1141 | U    | C5-C4-O4   | 5.90  | 143.61      | 125.90   |
| 17  | D     | 37   | U    | C5-C4-O4   | 5.89  | 143.56      | 125.90   |
| 20  | G     | 157  | LEU  | C-N-CD     | -5.87 | 100.93      | 125.00   |
| 17  | D     | 1358 | U    | C5-C4-O4   | 5.84  | 143.42      | 125.90   |
| 37  | X     | 81   | MET  | CG-SD-CE   | -5.83 | 88.07       | 100.90   |
| 22  | I     | 168  | TYR  | N-CA-CB    | 5.83  | 120.21      | 110.59   |
| 53  | n     | 176  | PRO  | N-CA-C     | 5.83  | 121.20      | 114.20   |
| 12  | AB    | 129  | ILE  | CA-C-N     | 5.83  | 132.67      | 121.54   |
| 12  | AB    | 129  | ILE  | C-N-CA     | 5.83  | 132.67      | 121.54   |
| 26  | M     | 55   | GLY  | CA-C-N     | 5.77  | 132.56      | 121.54   |
| 26  | M     | 55   | GLY  | C-N-CA     | 5.77  | 132.56      | 121.54   |
| 17  | D     | 884  | U    | N3-C4-O4   | -5.77 | 102.10      | 119.40   |
| 17  | D     | 827  | U    | C5-C4-O4   | 5.73  | 143.10      | 125.90   |
| 20  | G     | 154  | MET  | CA-CB-CG   | -5.73 | 102.64      | 114.10   |
| 14  | AE    | 853  | THR  | CA-C-N     | 5.71  | 130.97      | 122.74   |
| 14  | AE    | 853  | THR  | C-N-CA     | 5.71  | 130.97      | 122.74   |
| 22  | I     | 134  | MET  | CG-SD-CE   | -5.68 | 88.40       | 100.90   |
| 9   | 9     | 130  | PRO  | CA-N-CD    | -5.64 | 104.10      | 112.00   |
| 24  | K     | 45   | ARG  | CB-CG-CD   | -5.63 | 98.34       | 111.30   |
| 24  | K     | 45   | ARG  | CA-C-N     | 5.63  | 130.33      | 122.23   |
| 24  | K     | 45   | ARG  | C-N-CA     | 5.63  | 130.33      | 122.23   |
| 20  | G     | 154  | MET  | CG-SD-CE   | -5.62 | 88.52       | 100.90   |
| 59  | t     | 18   | ARG  | CG-CD-NE   | -5.57 | 99.75       | 112.00   |
| 12  | AB    | 151  | LYS  | CA-C-N     | 5.56  | 132.16      | 121.54   |
| 12  | AB    | 151  | LYS  | C-N-CA     | 5.56  | 132.16      | 121.54   |
| 40  | a     | 1141 | U    | N3-C4-O4   | -5.55 | 102.75      | 119.40   |
| 49  | j     | 11   | MET  | CB-CG-SD   | -5.50 | 96.19       | 112.70   |
| 14  | AE    | 1184 | ASP  | N-CA-C     | 5.45  | 121.85      | 109.81   |
| 61  | v     | 10   | ARG  | NE-CZ-NH1  | -5.44 | 116.06      | 121.50   |
| 9   | 9     | 129  | LEU  | C-N-CD     | -5.40 | 102.87      | 125.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 30  | Q     | 106  | ARG  | NE-CZ-NH1   | -5.36 | 116.14      | 121.50   |
| 62  | w     | 38   | LEU  | N-CA-C      | -5.34 | 105.20      | 112.35   |
| 55  | p     | 46   | ALA  | CA-C-N      | 5.25  | 131.57      | 121.54   |
| 55  | p     | 46   | ALA  | C-N-CA      | 5.25  | 131.57      | 121.54   |
| 24  | K     | 45   | ARG  | O-C-N       | -5.24 | 116.82      | 123.01   |
| 29  | P     | 88   | MET  | CG-SD-CE    | -5.24 | 89.37       | 100.90   |
| 38  | Y     | 5    | GLN  | CB-CA-C     | -5.24 | 100.00      | 110.42   |
| 8   | 7     | 10   | U    | C2'-C3'-O3' | 5.23  | 117.34      | 109.50   |
| 40  | a     | 2613 | U    | C5-C4-O4    | 5.21  | 141.52      | 125.90   |
| 38  | Y     | 5    | GLN  | CA-CB-CG    | 5.18  | 124.45      | 114.10   |
| 20  | G     | 158  | PRO  | N-CA-CB     | -5.17 | 97.95       | 103.38   |
| 22  | I     | 170  | GLU  | CB-CG-CD    | 5.15  | 121.35      | 112.60   |
| 40  | a     | 2334 | U    | C2'-C3'-O3' | -5.13 | 101.81      | 109.50   |
| 44  | e     | 25   | GLN  | CG-CD-NE2   | -5.12 | 108.72      | 116.40   |
| 40  | a     | 2602 | A    | C4'-C3'-O3' | 5.09  | 117.04      | 109.40   |
| 17  | D     | 884  | U    | C5-C4-O4    | 5.09  | 141.17      | 125.90   |
| 14  | AE    | 709  | ARG  | CA-C-N      | 5.08  | 135.44      | 126.45   |
| 14  | AE    | 709  | ARG  | C-N-CA      | 5.08  | 135.44      | 126.45   |
| 12  | AB    | 159  | PHE  | CA-CB-CG    | 5.07  | 118.87      | 113.80   |
| 47  | h     | 181  | MET  | CG-SD-CE    | -5.00 | 89.89       | 100.90   |

There are no chirality outliers.

All (36) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 9   | 9     | 107  | GLU  | Peptide |
| 9   | 9     | 79   | PRO  | Peptide |
| 9   | 9     | 92   | ALA  | Peptide |
| 12  | AB    | 106  | ASP  | Peptide |
| 12  | AB    | 116  | VAL  | Peptide |
| 12  | AB    | 117  | ILE  | Peptide |
| 12  | AB    | 128  | ALA  | Peptide |
| 12  | AB    | 137  | ALA  | Peptide |
| 12  | AB    | 140  | MET  | Peptide |
| 12  | AB    | 143  | LEU  | Peptide |
| 12  | AB    | 151  | LYS  | Peptide |
| 12  | AB    | 159  | PHE  | Peptide |
| 12  | AB    | 160  | ARG  | Peptide |
| 13  | AC    | 192  | VAL  | Peptide |
| 13  | AD    | 20   | SER  | Peptide |
| 14  | AE    | 1326 | GLN  | Peptide |
| 14  | AE    | 1344 | LEU  | Peptide |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 14  | AE    | 313 | GLY  | Peptide   |
| 14  | AE    | 416 | ILE  | Peptide   |
| 20  | G     | 19  | GLN  | Sidechain |
| 21  | H     | 124 | LEU  | Peptide   |
| 21  | H     | 171 | ARG  | Peptide   |
| 21  | H     | 274 | TYR  | Peptide   |
| 21  | H     | 81  | GLU  | Peptide   |
| 21  | H     | 82  | THR  | Peptide   |
| 22  | I     | 167 | TRP  | Mainchain |
| 24  | K     | 45  | ARG  | Mainchain |
| 24  | K     | 77  | ASN  | Peptide   |
| 28  | O     | 12  | ARG  | Peptide   |
| 37  | X     | 65  | VAL  | Peptide   |
| 38  | Y     | 5   | GLN  | Peptide   |
| 53  | n     | 176 | PRO  | Peptide   |
| 54  | o     | 31  | HIS  | Peptide   |
| 58  | s     | 74  | TYR  | Sidechain |
| 60  | u     | 35  | HIS  | Peptide   |
| 60  | u     | 62  | PRO  | Peptide   |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 816   | 839      | 839      | 54      | 0            |
| 2   | 1     | 857   | 922      | 922      | 68      | 0            |
| 3   | 2     | 746   | 811      | 811      | 61      | 0            |
| 4   | 3     | 788   | 844      | 844      | 45      | 0            |
| 5   | 4     | 753   | 780      | 780      | 88      | 0            |
| 6   | 5     | 726   | 0        | 392      | 110     | 0            |
| 7   | 6     | 703   | 0        | 396      | 35      | 0            |
| 8   | 7     | 792   | 0        | 392      | 109     | 0            |
| 9   | 9     | 1117  | 0        | 1155     | 257     | 0            |
| 10  | A     | 1620  | 826      | 827      | 109     | 0            |
| 10  | B     | 1620  | 814      | 827      | 111     | 0            |
| 11  | AA    | 10381 | 0        | 10390    | 234     | 0            |
| 12  | AB    | 1286  | 0        | 1300     | 345     | 0            |
| 13  | AC    | 1698  | 0        | 1718     | 11      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 13  | AD    | 1677  | 0        | 1713     | 28      | 0            |
| 14  | AE    | 10404 | 0        | 10626    | 269     | 0            |
| 15  | AF    | 650   | 0        | 658      | 15      | 0            |
| 16  | C     | 544   | 559      | 560      | 109     | 0            |
| 17  | D     | 32703 | 16423    | 16453    | 737     | 0            |
| 18  | E     | 669   | 719      | 719      | 82      | 0            |
| 19  | F     | 589   | 629      | 629      | 59      | 0            |
| 20  | G     | 1760  | 1785     | 1787     | 154     | 0            |
| 21  | H     | 1730  | 1454     | 1455     | 163     | 0            |
| 22  | I     | 1636  | 1710     | 1710     | 133     | 0            |
| 23  | J     | 1643  | 1707     | 1707     | 85      | 0            |
| 24  | K     | 1152  | 1196     | 1196     | 117     | 0            |
| 25  | L     | 848   | 846      | 846      | 104     | 0            |
| 26  | M     | 1181  | 1235     | 1238     | 123     | 0            |
| 27  | N     | 979   | 1031     | 1031     | 95      | 0            |
| 28  | O     | 1022  | 1070     | 1070     | 89      | 0            |
| 29  | P     | 790   | 831      | 831      | 137     | 0            |
| 30  | Q     | 877   | 887      | 887      | 96      | 0            |
| 31  | R     | 939   | 1001     | 1001     | 91      | 0            |
| 32  | S     | 805   | 844      | 844      | 76      | 0            |
| 33  | T     | 714   | 734      | 734      | 92      | 0            |
| 34  | U     | 649   | 666      | 666      | 63      | 0            |
| 35  | V     | 648   | 691      | 691      | 68      | 0            |
| 36  | W     | 663   | 688      | 688      | 47      | 0            |
| 37  | X     | 900   | 964      | 965      | 111     | 0            |
| 38  | Y     | 1032  | 0        | 1088     | 214     | 0            |
| 39  | Z     | 227   | 0        | 237      | 29      | 0            |
| 40  | a     | 61841 | 31077    | 31120    | 1318    | 0            |
| 41  | b     | 582   | 599      | 599      | 48      | 0            |
| 42  | c     | 625   | 652      | 652      | 33      | 0            |
| 43  | d     | 2569  | 1301     | 1301     | 43      | 0            |
| 44  | e     | 501   | 531      | 531      | 45      | 0            |
| 45  | f     | 448   | 488      | 488      | 38      | 0            |
| 46  | g     | 522   | 520      | 520      | 65      | 0            |
| 47  | h     | 2082  | 2154     | 2154     | 138     | 0            |
| 48  | i     | 444   | 459      | 458      | 48      | 0            |
| 49  | j     | 1565  | 1617     | 1616     | 123     | 0            |
| 50  | k     | 426   | 464      | 464      | 44      | 0            |
| 51  | l     | 1552  | 1619     | 1619     | 125     | 0            |
| 52  | m     | 377   | 418      | 418      | 30      | 0            |
| 53  | n     | 1410  | 1443     | 1444     | 155     | 0            |
| 54  | o     | 504   | 572      | 572      | 52      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 55  | p     | 1313   | 1358     | 1358     | 74      | 0            |
| 56  | q     | 302    | 343      | 343      | 25      | 0            |
| 57  | r     | 1111   | 1148     | 1148     | 52      | 0            |
| 58  | s     | 1129   | 1162     | 1162     | 122     | 0            |
| 59  | t     | 946    | 1023     | 1023     | 103     | 0            |
| 60  | u     | 1053   | 1129     | 1129     | 79      | 0            |
| 61  | v     | 1074   | 1157     | 1157     | 123     | 0            |
| 62  | w     | 951    | 994      | 994      | 103     | 0            |
| 63  | x     | 892    | 923      | 923      | 49      | 0            |
| 64  | y     | 917    | 962      | 962      | 52      | 0            |
| 65  | z     | 947    | 1020     | 1019     | 79      | 0            |
| 66  | AE    | 1      | 0        | 0        | 0       | 0            |
| 67  | AE    | 2      | 0        | 0        | 3       | 0            |
| All | All   | 177420 | 98639    | 128797   | 6796    | 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 22.

All (6796) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:K:45:ARG:CD    | 24:K:45:ARG:CG     | 1.75                     | 1.59              |
| 14:AE:79:LYS:HA   | 14:AE:81:ARG:CZ    | 1.26                     | 1.59              |
| 6:5:10:DT:C7      | 11:AA:62:TYR:CD2   | 1.84                     | 1.58              |
| 6:5:9:DG:H5'      | 11:AA:473:ARG:CB   | 1.29                     | 1.58              |
| 6:5:11:DA:C5'     | 12:AB:67:THR:HG22  | 1.20                     | 1.58              |
| 6:5:9:DG:C5'      | 11:AA:473:ARG:HB3  | 1.34                     | 1.56              |
| 12:AB:147:ASN:HB2 | 29:P:100:ILE:CG2   | 1.27                     | 1.56              |
| 6:5:10:DT:C5      | 11:AA:62:TYR:CD2   | 1.95                     | 1.54              |
| 65:z:74:ILE:CG1   | 65:z:74:ILE:CD1    | 1.81                     | 1.53              |
| 12:AB:147:ASN:CB  | 29:P:100:ILE:HG23  | 1.42                     | 1.49              |
| 14:AE:72:CYS:SG   | 67:AE:1502:ZN:ZN   | 1.03                     | 1.48              |
| 7:6:23:DC:C5'     | 14:AE:259:ARG:HH12 | 1.21                     | 1.47              |
| 6:5:10:DT:C6      | 11:AA:62:TYR:CE2   | 2.00                     | 1.46              |
| 6:5:10:DT:C5      | 11:AA:62:TYR:CE2   | 2.04                     | 1.45              |
| 14:AE:79:LYS:HA   | 14:AE:81:ARG:NH1   | 1.20                     | 1.45              |
| 12:AB:81:PHE:CD2  | 14:AE:293:ARG:NH1  | 1.77                     | 1.44              |
| 6:5:11:DA:P       | 12:AB:68:THR:HA    | 1.58                     | 1.42              |
| 11:AA:380:ALA:N   | 12:AB:65:HIS:CE1   | 1.84                     | 1.37              |
| 6:5:9:DG:OP2      | 11:AA:473:ARG:CB   | 1.73                     | 1.36              |
| 11:AA:481:LEU:CD2 | 12:AB:16:ARG:CD    | 2.02                     | 1.35              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:AA:377:THR:OG1 | 12:AB:62:GLU:HB3   | 1.20                     | 1.35              |
| 14:AE:79:LYS:CA   | 14:AE:81:ARG:NH1   | 1.90                     | 1.32              |
| 14:AE:79:LYS:CA   | 14:AE:81:ARG:CZ    | 2.06                     | 1.32              |
| 12:AB:81:PHE:CE1  | 14:AE:293:ARG:CB   | 1.92                     | 1.31              |
| 12:AB:81:PHE:CE1  | 14:AE:293:ARG:HB3  | 1.32                     | 1.31              |
| 12:AB:82:GLY:CA   | 14:AE:142:GLU:HB2  | 1.62                     | 1.30              |
| 6:5:10:DT:H1'     | 12:AB:71:ALA:N     | 1.21                     | 1.29              |
| 12:AB:51:PHE:HE2  | 14:AE:288:PRO:CG   | 1.44                     | 1.28              |
| 6:5:11:DA:C5'     | 12:AB:67:THR:CG2   | 2.12                     | 1.28              |
| 6:5:11:DA:C3'     | 12:AB:67:THR:HG21  | 1.63                     | 1.28              |
| 11:AA:377:THR:OG1 | 12:AB:62:GLU:CB    | 1.80                     | 1.28              |
| 14:AE:287:ALA:CB  | 14:AE:292:VAL:HG13 | 1.61                     | 1.28              |
| 11:AA:387:ASN:CG  | 11:AA:394:ARG:NH1  | 1.92                     | 1.27              |
| 6:5:11:DA:OP2     | 12:AB:68:THR:CA    | 1.81                     | 1.27              |
| 6:5:10:DT:C1'     | 12:AB:71:ALA:H     | 1.46                     | 1.26              |
| 14:AE:288:PRO:HD2 | 14:AE:291:ILE:CG2  | 1.66                     | 1.26              |
| 12:AB:123:PHE:CE1 | 29:P:85:ASP:HB3    | 1.51                     | 1.26              |
| 8:7:15:U:O2       | 15:AF:83:VAL:HG12  | 1.10                     | 1.24              |
| 8:7:11:U:H4'      | 24:K:20:ARG:NH2    | 1.50                     | 1.24              |
| 12:AB:81:PHE:HA   | 14:AE:141:PHE:O    | 1.27                     | 1.23              |
| 12:AB:123:PHE:CE1 | 29:P:85:ASP:CB     | 2.19                     | 1.23              |
| 12:AB:51:PHE:CE2  | 14:AE:288:PRO:CG   | 2.22                     | 1.23              |
| 6:5:9:DG:C5'      | 11:AA:473:ARG:CB   | 2.02                     | 1.22              |
| 6:5:11:DA:OP2     | 12:AB:68:THR:HA    | 1.36                     | 1.22              |
| 6:5:10:DT:H71     | 11:AA:62:TYR:CG    | 1.75                     | 1.21              |
| 6:5:11:DA:OP2     | 12:AB:68:THR:N     | 1.73                     | 1.21              |
| 7:6:23:DC:C5'     | 14:AE:259:ARG:NH1  | 2.05                     | 1.20              |
| 7:6:25:DT:OP1     | 11:AA:496:LYS:CA   | 1.80                     | 1.19              |
| 11:AA:380:ALA:N   | 12:AB:65:HIS:HE1   | 1.29                     | 1.18              |
| 55:p:159:GLY:O    | 55:p:163:ARG:NH1   | 1.77                     | 1.17              |
| 6:5:9:DG:C5'      | 11:AA:473:ARG:CG   | 2.22                     | 1.17              |
| 12:AB:148:LYS:NZ  | 29:P:102:LEU:HB3   | 1.58                     | 1.17              |
| 57:r:135:HIS:ND1  | 57:r:137:GLU:OE1   | 1.77                     | 1.16              |
| 6:5:10:DT:H73     | 11:AA:62:TYR:CD2   | 1.77                     | 1.14              |
| 6:5:9:DG:H5'      | 11:AA:473:ARG:CG   | 1.76                     | 1.13              |
| 7:6:25:DT:C3'     | 11:AA:496:LYS:HG3  | 1.74                     | 1.13              |
| 12:AB:82:GLY:HA2  | 14:AE:142:GLU:HB2  | 1.13                     | 1.13              |
| 37:X:81:MET:HE1   | 37:X:92:ARG:HB3    | 1.20                     | 1.13              |
| 40:a:2335:A:OP2   | 63:x:13:ARG:NE     | 1.81                     | 1.13              |
| 6:5:10:DT:O3'     | 12:AB:67:THR:O     | 1.67                     | 1.12              |
| 11:AA:387:ASN:CG  | 11:AA:394:ARG:HH11 | 1.55                     | 1.13              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:L:9:MET:HE1    | 25:L:85:ILE:HB     | 1.17                     | 1.12              |
| 6:5:9:DG:OP2      | 11:AA:473:ARG:HB2  | 0.97                     | 1.12              |
| 10:A:76:A:O2'     | 40:a:2394:C:N3     | 1.81                     | 1.12              |
| 10:B:75:C:OP2     | 40:a:2602:A:O2'    | 1.68                     | 1.12              |
| 12:AB:102:LYS:CE  | 14:AE:285:LEU:HG   | 1.79                     | 1.12              |
| 6:5:10:DT:C7      | 11:AA:62:TYR:CG    | 2.31                     | 1.12              |
| 36:W:40:ILE:HD13  | 36:W:66:MET:SD     | 1.89                     | 1.12              |
| 12:AB:54:TYR:CE2  | 14:AE:291:ILE:HG23 | 1.84                     | 1.12              |
| 14:AE:287:ALA:HB2 | 14:AE:292:VAL:CG1  | 1.78                     | 1.12              |
| 35:V:7:THR:OG1    | 35:V:60:GLU:OE2    | 1.66                     | 1.12              |
| 45:f:4:THR:OG1    | 45:f:37:GLU:OE2    | 1.68                     | 1.12              |
| 12:AB:123:PHE:HZ  | 29:P:82:LYS:HA     | 1.10                     | 1.11              |
| 57:r:135:HIS:HD1  | 57:r:137:GLU:CD    | 1.58                     | 1.11              |
| 12:AB:81:PHE:CE2  | 14:AE:293:ARG:NH1  | 1.88                     | 1.10              |
| 12:AB:123:PHE:CE2 | 29:P:81:GLU:HG2    | 1.86                     | 1.10              |
| 12:AB:147:ASN:CG  | 29:P:100:ILE:HG23  | 1.75                     | 1.10              |
| 38:Y:96:LYS:HE3   | 38:Y:136:GLY:HA3   | 1.29                     | 1.10              |
| 6:5:10:DT:H71     | 11:AA:62:TYR:CD2   | 1.77                     | 1.10              |
| 12:AB:28:CYS:HA   | 12:AB:56:PHE:O     | 1.52                     | 1.10              |
| 12:AB:148:LYS:HZ1 | 29:P:102:LEU:CB    | 1.66                     | 1.09              |
| 8:7:11:U:C4'      | 24:K:20:ARG:NH2    | 2.16                     | 1.09              |
| 12:AB:138:ARG:HA  | 12:AB:154:VAL:O    | 1.50                     | 1.09              |
| 38:Y:5:GLN:HG2    | 38:Y:61:TYR:CE1    | 1.87                     | 1.09              |
| 7:6:23:DC:H5''    | 14:AE:259:ARG:HH12 | 1.14                     | 1.09              |
| 14:AE:79:LYS:HA   | 14:AE:81:ARG:NH2   | 1.66                     | 1.09              |
| 6:5:9:DG:H5'      | 11:AA:473:ARG:HG3  | 1.09                     | 1.09              |
| 12:AB:147:ASN:CB  | 29:P:100:ILE:CG2   | 2.11                     | 1.08              |
| 60:u:122:VAL:HG12 | 60:u:125:LEU:HD21  | 1.35                     | 1.08              |
| 8:7:15:U:O2       | 15:AF:83:VAL:CG1   | 2.00                     | 1.08              |
| 12:AB:51:PHE:CZ   | 14:AE:288:PRO:HD3  | 1.87                     | 1.08              |
| 14:AE:288:PRO:HD2 | 14:AE:291:ILE:HG21 | 1.10                     | 1.08              |
| 6:5:9:DG:C5'      | 11:AA:473:ARG:HG3  | 1.82                     | 1.08              |
| 6:5:11:DA:H5'     | 12:AB:67:THR:HG22  | 1.13                     | 1.08              |
| 52:m:22:MET:O     | 52:m:28:ARG:NH1    | 1.87                     | 1.08              |
| 11:AA:469:VAL:O   | 11:AA:473:ARG:HG2  | 1.53                     | 1.08              |
| 9:9:46:ARG:HG3    | 9:9:94:ARG:HH21    | 1.12                     | 1.07              |
| 12:AB:147:ASN:HB2 | 29:P:100:ILE:HG21  | 1.13                     | 1.07              |
| 9:9:50:VAL:HG22   | 38:Y:119:ALA:HB3   | 1.33                     | 1.07              |
| 12:AB:82:GLY:HA2  | 14:AE:142:GLU:CB   | 1.85                     | 1.07              |
| 17:D:1309:G:OP2   | 37:X:98:ARG:NE     | 1.88                     | 1.07              |
| 7:6:23:DC:O5'     | 14:AE:259:ARG:NH1  | 1.87                     | 1.06              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:AE:287:ALA:HB2  | 14:AE:292:VAL:HG13 | 1.08                     | 1.06              |
| 12:AB:123:PHE:CZ   | 29:P:82:LYS:HA     | 1.88                     | 1.06              |
| 26:M:4:ARG:HG3     | 26:M:5:ARG:HG3     | 1.33                     | 1.06              |
| 12:AB:123:PHE:HE2  | 29:P:81:GLU:HG2    | 1.02                     | 1.06              |
| 38:Y:56:VAL:HA     | 38:Y:71:LYS:HZ1    | 1.21                     | 1.05              |
| 12:AB:147:ASN:ND2  | 29:P:100:ILE:HG12  | 1.70                     | 1.05              |
| 6:5:11:DA:H3'      | 12:AB:67:THR:HG21  | 1.05                     | 1.05              |
| 38:Y:14:ALA:HB1    | 38:Y:50:LYS:HD2    | 1.37                     | 1.05              |
| 8:7:11:U:O2'       | 24:K:33:PHE:CE1    | 2.10                     | 1.04              |
| 19:F:25:LYS:NZ     | 21:H:336:ASP:OD1   | 1.90                     | 1.04              |
| 7:6:18:DT:H3       | 8:7:34:A:N6        | 1.55                     | 1.04              |
| 25:L:9:MET:HE1     | 25:L:85:ILE:CB     | 1.86                     | 1.04              |
| 19:F:37:PHE:HB2    | 30:Q:126:LYS:HE2   | 1.35                     | 1.04              |
| 9:9:103:ASN:ND2    | 9:9:107:GLU:OE2    | 1.91                     | 1.04              |
| 9:9:136:ILE:HD12   | 9:9:139:LEU:HD12   | 1.38                     | 1.04              |
| 46:g:58:ASP:OD1    | 46:g:62:LYS:NZ     | 1.90                     | 1.04              |
| 49:j:184:ARG:NH2   | 64:y:7:GLN:OE1     | 1.90                     | 1.03              |
| 49:j:179:ARG:NH1   | 49:j:180:VAL:O     | 1.92                     | 1.03              |
| 55:p:149:ARG:NH2   | 55:p:152:ARG:O     | 1.91                     | 1.03              |
| 12:AB:146:ILE:HD11 | 29:P:88:MET:HA     | 1.38                     | 1.03              |
| 38:Y:93:ASN:HA     | 38:Y:135:MET:CE    | 1.89                     | 1.03              |
| 51:l:1:MET:HE2     | 51:l:16:GLU:HA     | 1.40                     | 1.03              |
| 64:y:51:ARG:NH1    | 64:y:56:HIS:O      | 1.91                     | 1.02              |
| 12:AB:81:PHE:CA    | 14:AE:141:PHE:O    | 2.06                     | 1.02              |
| 12:AB:102:LYS:HE2  | 14:AE:285:LEU:HG   | 1.08                     | 1.02              |
| 6:5:10:DT:C1'      | 12:AB:71:ALA:N     | 2.10                     | 1.02              |
| 8:7:4:U:O2'        | 17:D:1403:C:O2     | 1.75                     | 1.02              |
| 22:I:123:GLN:OE1   | 22:I:126:ARG:NH2   | 1.91                     | 1.02              |
| 25:L:42:TRP:CH2    | 25:L:102:MET:HG3   | 1.94                     | 1.02              |
| 9:9:3:LEU:HD12     | 9:9:4:ASN:H        | 1.25                     | 1.02              |
| 9:9:48:ALA:HB3     | 9:9:51:TYR:HE1     | 1.20                     | 1.02              |
| 12:AB:51:PHE:HE2   | 14:AE:288:PRO:HG2  | 1.20                     | 1.02              |
| 17:D:564:C:OP2     | 31:R:12:ARG:NH2    | 1.91                     | 1.02              |
| 9:9:31:ARG:NH1     | 40:a:1054:A:O4'    | 1.91                     | 1.01              |
| 58:s:72:LYS:HD3    | 58:s:74:TYR:OH     | 1.59                     | 1.01              |
| 22:I:152:GLU:OE2   | 22:I:154:SER:OG    | 1.77                     | 1.01              |
| 8:7:3:G:H5''       | 17:D:1500:A:N6     | 1.75                     | 1.01              |
| 12:AB:102:LYS:HE2  | 14:AE:285:LEU:CG   | 1.90                     | 1.01              |
| 9:9:43:LYS:HG3     | 9:9:46:ARG:HH12    | 1.22                     | 1.00              |
| 10:B:30:G:HO2'     | 17:D:1339:A:H2     | 1.04                     | 1.00              |
| 6:5:11:DA:H3'      | 12:AB:67:THR:CG2   | 1.90                     | 1.00              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:5:11:DA:H5''     | 12:AB:67:THR:CG2   | 1.86                     | 1.00              |
| 9:9:88:HIS:HB3     | 9:9:89:PRO:HD3     | 1.44                     | 1.00              |
| 14:AE:70:CYS:SG    | 14:AE:85:CYS:SG    | 2.60                     | 1.00              |
| 38:Y:60:VAL:HG22   | 38:Y:66:PHE:HB3    | 1.44                     | 1.00              |
| 51:l:1:MET:HE1     | 51:l:20:GLY:HA3    | 1.43                     | 1.00              |
| 38:Y:93:ASN:HA     | 38:Y:135:MET:HE1   | 1.00                     | 0.99              |
| 12:AB:82:GLY:CA    | 14:AE:142:GLU:CB   | 2.39                     | 0.99              |
| 6:5:11:DA:P        | 12:AB:68:THR:CA    | 2.45                     | 0.99              |
| 9:9:30:SER:O       | 9:9:31:ARG:NE      | 1.94                     | 0.99              |
| 11:AA:481:LEU:HD23 | 12:AB:16:ARG:CD    | 1.87                     | 0.99              |
| 7:6:25:DT:H3'      | 11:AA:496:LYS:HG3  | 1.41                     | 0.99              |
| 14:AE:70:CYS:SG    | 14:AE:72:CYS:SG    | 2.61                     | 0.99              |
| 17:D:377:G:OP1     | 34:U:5:ARG:NH1     | 1.94                     | 0.99              |
| 32:S:86:GLU:OE1    | 32:S:90:ARG:NH1    | 1.96                     | 0.99              |
| 7:6:18:DT:H3       | 8:7:34:A:H61       | 1.05                     | 0.99              |
| 12:AB:148:LYS:CE   | 29:P:102:LEU:HB3   | 1.92                     | 0.98              |
| 25:L:42:TRP:HH2    | 25:L:102:MET:HG3   | 1.25                     | 0.98              |
| 57:r:38:PRO:O      | 57:r:43:ASN:ND2    | 1.96                     | 0.98              |
| 20:G:49:MET:HE1    | 20:G:201:PRO:HD3   | 1.42                     | 0.98              |
| 12:AB:51:PHE:CE2   | 14:AE:288:PRO:HG3  | 1.99                     | 0.98              |
| 14:AE:288:PRO:CD   | 14:AE:291:ILE:HG21 | 1.92                     | 0.98              |
| 12:AB:140:MET:N    | 12:AB:152:HIS:O    | 1.96                     | 0.97              |
| 20:G:154:MET:HE2   | 20:G:158:PRO:HD3   | 1.44                     | 0.97              |
| 32:S:92:GLU:OE1    | 32:S:92:GLU:N      | 1.97                     | 0.97              |
| 58:s:12:LYS:NZ     | 58:s:14:ASP:OD1    | 1.96                     | 0.97              |
| 6:5:10:DT:O5'      | 11:AA:62:TYR:OH    | 1.80                     | 0.97              |
| 8:7:11:U:H4'       | 24:K:20:ARG:HH22   | 1.18                     | 0.97              |
| 11:AA:481:LEU:HD21 | 12:AB:16:ARG:CD    | 1.60                     | 0.97              |
| 9:9:58:THR:HG21    | 9:9:81:LEU:HD23    | 1.48                     | 0.96              |
| 12:AB:6:LEU:HD13   | 14:AE:291:ILE:HD11 | 1.46                     | 0.96              |
| 38:Y:93:ASN:CA     | 38:Y:135:MET:HE1   | 1.94                     | 0.96              |
| 6:5:11:DA:H5'      | 12:AB:67:THR:CG2   | 1.81                     | 0.96              |
| 14:AE:287:ALA:CB   | 14:AE:292:VAL:CG1  | 2.38                     | 0.96              |
| 6:5:11:DA:C3'      | 12:AB:67:THR:CG2   | 2.42                     | 0.96              |
| 9:9:95:LEU:HD13    | 9:9:98:GLU:OE2     | 1.65                     | 0.96              |
| 11:AA:387:ASN:ND2  | 11:AA:394:ARG:HH12 | 1.61                     | 0.96              |
| 17:D:562:U:O2'     | 31:R:14:ARG:NH1    | 1.98                     | 0.96              |
| 40:a:2093:G:OP1    | 57:r:22:LYS:NZ     | 1.98                     | 0.96              |
| 63:x:111:ARG:NH2   | 63:x:117:PHE:OXT   | 1.99                     | 0.96              |
| 12:AB:147:ASN:ND2  | 29:P:100:ILE:HG23  | 1.80                     | 0.96              |
| 17:D:1344:C:OP1    | 28:O:124:ARG:NH1   | 1.98                     | 0.95              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:7:2:U:P          | 17:D:1505:G:H8    | 1.88                     | 0.95              |
| 38:Y:75:ALA:HB2    | 38:Y:112:LYS:HE3  | 1.48                     | 0.95              |
| 9:9:3:LEU:HD12     | 9:9:4:ASN:N       | 1.82                     | 0.95              |
| 9:9:61:ARG:NH1     | 40:a:1047:G:N7    | 2.15                     | 0.95              |
| 12:AB:51:PHE:CE2   | 14:AE:288:PRO:CD  | 2.48                     | 0.95              |
| 12:AB:82:GLY:N     | 14:AE:142:GLU:CB  | 2.30                     | 0.95              |
| 11:AA:387:ASN:ND2  | 11:AA:394:ARG:NH1 | 2.15                     | 0.94              |
| 6:5:11:DA:H5''     | 12:AB:67:THR:HG22 | 0.98                     | 0.94              |
| 9:9:23:LEU:HD13    | 9:9:92:ALA:CB     | 1.98                     | 0.94              |
| 14:AE:85:CYS:HG    | 67:AE:1502:ZN:ZN  | 0.75                     | 0.94              |
| 38:Y:5:GLN:HG2     | 38:Y:61:TYR:HE1   | 1.31                     | 0.94              |
| 35:V:7:THR:OG1     | 35:V:61:ILE:O     | 1.85                     | 0.94              |
| 40:a:30:G:OP2      | 65:z:5:LYS:NZ     | 2.00                     | 0.94              |
| 7:6:25:DT:OP1      | 11:AA:496:LYS:HA  | 1.12                     | 0.94              |
| 9:9:23:LEU:HD13    | 9:9:92:ALA:HB1    | 1.49                     | 0.94              |
| 12:AB:146:ILE:HD11 | 29:P:88:MET:HG3   | 1.50                     | 0.94              |
| 22:I:164:ARG:NH2   | 22:I:166:GLU:OE2  | 1.99                     | 0.94              |
| 6:5:10:DT:C6       | 11:AA:62:TYR:HE2  | 1.85                     | 0.93              |
| 9:9:31:ARG:HD2     | 40:a:1053:C:O2'   | 1.66                     | 0.93              |
| 38:Y:14:ALA:O      | 38:Y:50:LYS:HE3   | 1.67                     | 0.93              |
| 39:Z:14:MET:HB3    | 39:Z:17:MET:HG2   | 1.46                     | 0.93              |
| 11:AA:481:LEU:HD21 | 12:AB:16:ARG:HD3  | 1.48                     | 0.93              |
| 55:p:38:ASN:ND2    | 55:p:64:GLN:OE1   | 2.00                     | 0.93              |
| 11:AA:481:LEU:CD2  | 12:AB:16:ARG:HD3  | 1.99                     | 0.93              |
| 10:B:76:A:N3       | 40:a:2493:U:H4'   | 1.84                     | 0.93              |
| 38:Y:33:ASN:HB3    | 38:Y:36:GLU:HG2   | 1.48                     | 0.93              |
| 17:D:526:C:OP2     | 31:R:88:LYS:NZ    | 2.01                     | 0.93              |
| 9:9:88:HIS:HB3     | 9:9:89:PRO:CD     | 1.97                     | 0.93              |
| 25:L:9:MET:CE      | 25:L:85:ILE:HB    | 1.97                     | 0.93              |
| 1:0:18:GLN:N       | 1:0:18:GLN:OE1    | 2.01                     | 0.92              |
| 6:5:11:DA:OP2      | 12:AB:67:THR:C    | 2.11                     | 0.92              |
| 59:t:90:ASN:OD1    | 59:t:91:SER:N     | 2.02                     | 0.92              |
| 9:9:50:VAL:HG22    | 38:Y:119:ALA:CB   | 1.98                     | 0.92              |
| 12:AB:81:PHE:CE1   | 14:AE:293:ARG:HB2 | 1.91                     | 0.92              |
| 14:AE:59:ALA:CB    | 14:AE:71:LEU:HD21 | 1.99                     | 0.92              |
| 12:AB:123:PHE:HZ   | 29:P:82:LYS:CA    | 1.82                     | 0.92              |
| 12:AB:140:MET:C    | 12:AB:152:HIS:O   | 2.13                     | 0.92              |
| 6:5:9:DG:P         | 11:AA:473:ARG:HB2 | 2.10                     | 0.92              |
| 12:AB:148:LYS:HZ1  | 29:P:102:LEU:HB3  | 1.16                     | 0.92              |
| 6:5:9:DG:OP2       | 11:AA:473:ARG:CG  | 2.16                     | 0.91              |
| 6:5:10:DT:C7       | 11:AA:62:TYR:HD2  | 1.69                     | 0.91              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 17:D:1526:G:N7    | 19:F:40:LYS:NZ      | 2.18                     | 0.91              |
| 40:a:2293:G:OP1   | 63:x:94:ARG:NH1     | 2.04                     | 0.91              |
| 12:AB:148:LYS:HZ1 | 29:P:102:LEU:CG     | 1.83                     | 0.91              |
| 40:a:2682:A:O4'   | 49:j:11:MET:SD      | 2.29                     | 0.91              |
| 26:M:50:LEU:HD21  | 26:M:121:ALA:HA     | 1.52                     | 0.91              |
| 35:V:27:ARG:NH1   | 35:V:42:THR:OG1     | 2.03                     | 0.91              |
| 10:B:38:A:H4'     | 17:D:790:A:O4'      | 1.71                     | 0.91              |
| 8:7:2:U:P         | 17:D:1505:G:C8      | 2.64                     | 0.91              |
| 9:9:92:ALA:O      | 9:9:129:LEU:HD13    | 1.71                     | 0.91              |
| 12:AB:3:SER:O     | 12:AB:58:GLU:HA     | 1.71                     | 0.91              |
| 8:7:29:U:H5'      | 11:AA:1259:LEU:HD21 | 1.52                     | 0.90              |
| 12:AB:81:PHE:HD2  | 14:AE:293:ARG:NH1   | 1.35                     | 0.90              |
| 38:Y:79:LEU:HD21  | 38:Y:105:LEU:HD21   | 1.52                     | 0.90              |
| 11:AA:380:ALA:H   | 12:AB:65:HIS:CE1    | 1.61                     | 0.90              |
| 30:Q:51:GLY:O     | 30:Q:56:ARG:NH2     | 2.03                     | 0.90              |
| 24:K:45:ARG:CD    | 24:K:45:ARG:CB      | 2.49                     | 0.90              |
| 46:g:27:THR:OG1   | 53:n:140:GLU:OE1    | 1.88                     | 0.90              |
| 63:x:36:TYR:OH    | 63:x:38:GLN:NE2     | 2.05                     | 0.90              |
| 61:v:111:GLU:O    | 61:v:114:ARG:HG2    | 1.71                     | 0.90              |
| 64:y:89:ARG:NE    | 64:y:113:ARG:O      | 2.05                     | 0.90              |
| 7:6:25:DT:H2'     | 11:AA:496:LYS:HE3   | 1.51                     | 0.90              |
| 40:a:1818:U:OP2   | 47:h:156:ARG:NH1    | 2.03                     | 0.90              |
| 40:a:1042:G:HO2'  | 40:a:1043:C:H6      | 1.10                     | 0.90              |
| 40:a:2393:U:OP1   | 54:o:30:ARG:NE      | 2.05                     | 0.90              |
| 16:C:60:LYS:HZ2   | 17:D:734:G:C2'      | 1.85                     | 0.89              |
| 6:5:11:DA:P       | 12:AB:67:THR:O      | 2.30                     | 0.89              |
| 12:AB:142:LEU:HA  | 12:AB:150:ILE:O     | 1.72                     | 0.89              |
| 17:D:1439:G:OP1   | 18:E:33:LYS:NZ      | 2.05                     | 0.89              |
| 19:F:31:GLU:OE2   | 19:F:35:ARG:NE      | 2.06                     | 0.89              |
| 44:e:23:ARG:NH1   | 44:e:24:GLU:OE2     | 2.06                     | 0.89              |
| 9:9:8:LYS:O       | 9:9:12:VAL:HG23     | 1.73                     | 0.89              |
| 12:AB:51:PHE:HE2  | 14:AE:288:PRO:CD    | 1.86                     | 0.89              |
| 16:C:38:LYS:NZ    | 17:D:718:A:N1       | 2.19                     | 0.89              |
| 26:M:66:LEU:HD13  | 26:M:101:MET:CE     | 2.02                     | 0.89              |
| 46:g:16:CYS:HB2   | 46:g:37:CYS:HB3     | 1.54                     | 0.89              |
| 6:5:10:DT:H2''    | 12:AB:70:ASN:N      | 1.87                     | 0.89              |
| 12:AB:123:PHE:CZ  | 29:P:85:ASP:HB3     | 2.07                     | 0.89              |
| 30:Q:15:GLN:NE2   | 30:Q:76:GLU:O       | 2.06                     | 0.89              |
| 16:C:60:LYS:NZ    | 17:D:735:C:O4'      | 2.06                     | 0.89              |
| 60:u:93:ASN:OD1   | 60:u:94:THR:N       | 2.05                     | 0.89              |
| 14:AE:59:ALA:CB   | 14:AE:71:LEU:CD2    | 2.51                     | 0.89              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:Y:45:THR:CG2   | 38:Y:50:LYS:HD3    | 2.02                     | 0.89              |
| 38:Y:129:GLU:HB3  | 38:Y:133:ARG:NH1   | 1.87                     | 0.89              |
| 3:2:54:GLU:OE1    | 3:2:91:GLN:NE2     | 2.06                     | 0.88              |
| 17:D:280:C:O2     | 35:V:40:ARG:CZ     | 2.21                     | 0.88              |
| 32:S:90:ARG:HG3   | 32:S:92:GLU:OE1    | 1.73                     | 0.88              |
| 10:A:76:A:N6      | 40:a:2422:C:O4'    | 2.06                     | 0.88              |
| 14:AE:79:LYS:HA   | 14:AE:81:ARG:HH12  | 1.32                     | 0.88              |
| 12:AB:82:GLY:N    | 14:AE:142:GLU:HB3  | 1.87                     | 0.88              |
| 40:a:585:G:N7     | 65:z:6:ARG:NH1     | 2.21                     | 0.88              |
| 51:l:170:ARG:NH1  | 51:l:174:GLY:O     | 2.05                     | 0.88              |
| 40:a:2756:U:OP2   | 56:q:19:ARG:NE     | 2.06                     | 0.88              |
| 38:Y:100:ILE:HD12 | 38:Y:105:LEU:HD11  | 1.54                     | 0.88              |
| 40:a:78:U:OP1     | 44:e:4:LYS:NZ      | 2.06                     | 0.88              |
| 40:a:404:A:O2'    | 40:a:405:U:OP2     | 1.90                     | 0.88              |
| 26:M:13:LEU:HD12  | 26:M:14:PRO:HD2    | 1.54                     | 0.88              |
| 26:M:4:ARG:HG2    | 26:M:5:ARG:CZ      | 2.03                     | 0.88              |
| 17:D:545:C:H5'    | 23:J:69:GLU:HG3    | 1.55                     | 0.88              |
| 16:C:27:ALA:O     | 16:C:30:LYS:HG2    | 1.74                     | 0.87              |
| 27:N:5:ASP:OD2    | 27:N:77:ARG:NH1    | 2.07                     | 0.87              |
| 12:AB:6:LEU:CD1   | 14:AE:291:ILE:HD11 | 2.05                     | 0.87              |
| 51:l:170:ARG:NH1  | 51:l:176:ASP:OD1   | 2.07                     | 0.87              |
| 58:s:98:GLU:OE2   | 58:s:126:ALA:N     | 2.07                     | 0.87              |
| 14:AE:78:LEU:C    | 14:AE:81:ARG:HH11  | 1.79                     | 0.87              |
| 58:s:13:ARG:NH1   | 58:s:49:ASP:O      | 2.07                     | 0.87              |
| 38:Y:99:LYS:HD2   | 38:Y:140:GLU:OE1   | 1.75                     | 0.87              |
| 23:J:67:VAL:HB    | 23:J:72:PHE:CZ     | 2.09                     | 0.87              |
| 43:d:55:U:H1'     | 53:n:26:MET:HE2    | 1.57                     | 0.87              |
| 62:w:24:MET:HA    | 62:w:24:MET:HE3    | 1.54                     | 0.86              |
| 6:5:10:DT:O4'     | 11:AA:62:TYR:OH    | 1.93                     | 0.86              |
| 38:Y:15:GLY:HA2   | 38:Y:50:LYS:HG3    | 1.57                     | 0.86              |
| 12:AB:81:PHE:HE1  | 14:AE:293:ARG:CB   | 1.55                     | 0.86              |
| 40:a:2780:G:OP2   | 58:s:120:ARG:NH1   | 2.07                     | 0.86              |
| 22:I:58:GLU:OE1   | 22:I:65:ARG:NH1    | 2.08                     | 0.86              |
| 37:X:81:MET:HE2   | 40:a:888:C:C5      | 2.09                     | 0.86              |
| 7:6:25:DT:C2'     | 11:AA:496:LYS:HG3  | 2.05                     | 0.86              |
| 35:V:77:ARG:NH2   | 35:V:78:VAL:O      | 2.08                     | 0.86              |
| 58:s:37:ARG:HA    | 58:s:118:MET:HE3   | 1.54                     | 0.86              |
| 14:AE:79:LYS:N    | 14:AE:81:ARG:NH1   | 2.22                     | 0.86              |
| 25:L:102:MET:N    | 25:L:102:MET:SD    | 2.46                     | 0.86              |
| 38:Y:48:ILE:HG13  | 38:Y:49:GLU:H      | 1.41                     | 0.86              |
| 38:Y:129:GLU:HB3  | 38:Y:133:ARG:HH12  | 1.38                     | 0.86              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:AB:51:PHE:CE2  | 14:AE:288:PRO:HD3  | 2.08                     | 0.85              |
| 61:v:95:LEU:O     | 61:v:100:LYS:NZ    | 2.08                     | 0.85              |
| 12:AB:121:GLY:HA3 | 12:AB:162:LEU:HD12 | 1.57                     | 0.85              |
| 29:P:85:ASP:HA    | 29:P:88:MET:HE1    | 1.58                     | 0.85              |
| 61:v:77:PRO:HG2   | 61:v:80:VAL:HG21   | 1.57                     | 0.85              |
| 1:0:87:GLN:NE2    | 1:0:88:GLY:O       | 2.09                     | 0.85              |
| 35:V:25:ILE:O     | 35:V:27:ARG:NH2    | 2.10                     | 0.85              |
| 12:AB:141:LEU:HA  | 12:AB:153:SER:N    | 1.92                     | 0.85              |
| 46:g:26:SER:OG    | 53:n:140:GLU:OE2   | 1.94                     | 0.85              |
| 9:9:58:THR:CG2    | 9:9:81:LEU:HD23    | 2.06                     | 0.85              |
| 12:AB:123:PHE:CZ  | 29:P:81:GLU:O      | 2.30                     | 0.85              |
| 53:n:23:ASN:OD1   | 53:n:24:SER:N      | 2.09                     | 0.85              |
| 28:O:84:THR:HG21  | 28:O:103:PHE:HB3   | 1.59                     | 0.85              |
| 41:b:36:ILE:HG21  | 41:b:39:ARG:HD3    | 1.59                     | 0.85              |
| 38:Y:100:ILE:HD12 | 38:Y:105:LEU:CD1   | 2.05                     | 0.84              |
| 62:w:38:LEU:HD13  | 62:w:111:ALA:HB2   | 1.59                     | 0.84              |
| 1:0:68:ARG:NH1    | 40:a:1223:G:OP1    | 2.10                     | 0.84              |
| 12:AB:148:LYS:NZ  | 29:P:102:LEU:HD23  | 1.91                     | 0.84              |
| 37:X:81:MET:CE    | 37:X:92:ARG:HB3    | 2.06                     | 0.84              |
| 6:5:10:DT:C2      | 12:AB:72:THR:OG1   | 2.30                     | 0.84              |
| 18:E:9:LYS:O      | 18:E:13:GLN:NE2    | 2.10                     | 0.84              |
| 60:u:90:VAL:HG13  | 60:u:95:LEU:HD21   | 1.57                     | 0.84              |
| 5:4:58:SER:OG     | 5:4:59:GLU:OE1     | 1.95                     | 0.84              |
| 38:Y:75:ALA:CB    | 38:Y:112:LYS:HE3   | 2.07                     | 0.84              |
| 14:AE:287:ALA:HB1 | 14:AE:292:VAL:HG13 | 1.60                     | 0.84              |
| 49:j:55:LYS:HZ3   | 49:j:59:ARG:HB3    | 1.43                     | 0.84              |
| 38:Y:96:LYS:CE    | 38:Y:136:GLY:HA3   | 2.08                     | 0.84              |
| 8:7:2:U:OP2       | 17:D:1505:G:C8     | 2.30                     | 0.83              |
| 55:p:121:ILE:HD12 | 55:p:141:ILE:HG22  | 1.60                     | 0.83              |
| 6:5:10:DT:C6      | 11:AA:62:TYR:CZ    | 2.66                     | 0.83              |
| 12:AB:141:LEU:HB3 | 12:AB:143:LEU:HD12 | 1.60                     | 0.83              |
| 17:D:742:G:OP1    | 33:T:58:ARG:NH2    | 2.12                     | 0.83              |
| 58:s:102:GLU:OE1  | 58:s:102:GLU:N     | 2.10                     | 0.83              |
| 61:v:7:THR:OG1    | 61:v:10:ARG:NH1    | 2.11                     | 0.83              |
| 12:AB:51:PHE:HZ   | 14:AE:288:PRO:HD3  | 1.39                     | 0.83              |
| 6:5:9:DG:P        | 11:AA:473:ARG:CB   | 2.66                     | 0.83              |
| 9:9:43:LYS:O      | 9:9:46:ARG:HG2     | 1.78                     | 0.83              |
| 40:a:2682:A:O2'   | 49:j:13:ARG:NE     | 2.12                     | 0.83              |
| 6:5:11:DA:C2'     | 12:AB:67:THR:HG21  | 2.08                     | 0.83              |
| 38:Y:116:MET:HG2  | 38:Y:124:MET:HG2   | 1.59                     | 0.83              |
| 57:r:137:GLU:HG2  | 57:r:138:VAL:HG23  | 1.61                     | 0.83              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:z:78:LYS:HD3    | 65:z:117:LEU:CD2   | 2.09                     | 0.83              |
| 37:X:81:MET:HE1    | 37:X:92:ARG:CB     | 2.08                     | 0.83              |
| 60:u:122:VAL:CG1   | 60:u:125:LEU:HD21  | 2.07                     | 0.83              |
| 8:7:3:G:C5'        | 17:D:1500:A:H62    | 1.92                     | 0.83              |
| 47:h:175:ARG:HG3   | 47:h:181:MET:HE1   | 1.58                     | 0.83              |
| 49:j:152:PRO:HG3   | 49:j:156:PHE:CZ    | 2.14                     | 0.83              |
| 65:z:74:ILE:HD11   | 65:z:79:PHE:HA     | 1.60                     | 0.83              |
| 22:I:22:TRP:CZ3    | 22:I:24:ALA:HB2    | 2.14                     | 0.83              |
| 11:AA:377:THR:CB   | 12:AB:62:GLU:HB3   | 2.08                     | 0.82              |
| 12:AB:38:ILE:HG12  | 12:AB:43:ARG:HG2   | 1.61                     | 0.82              |
| 38:Y:74:PRO:HG2    | 38:Y:77:VAL:HB     | 1.60                     | 0.82              |
| 10:A:33:U:OP1      | 26:M:77:SER:OG     | 1.95                     | 0.82              |
| 11:AA:481:LEU:HD23 | 12:AB:16:ARG:HD2   | 1.60                     | 0.82              |
| 40:a:2393:U:H5''   | 54:o:30:ARG:CZ     | 2.09                     | 0.82              |
| 11:AA:380:ALA:H    | 12:AB:65:HIS:HE1   | 1.00                     | 0.82              |
| 40:a:1257:C:H4'    | 51:l:78:TRP:CE2    | 2.14                     | 0.82              |
| 40:a:2356:U:H5''   | 41:b:20:ARG:HD2    | 1.61                     | 0.82              |
| 8:7:24:U:OP1       | 11:AA:1299:ASN:ND2 | 2.13                     | 0.82              |
| 9:9:43:LYS:HG3     | 9:9:46:ARG:NH1     | 1.94                     | 0.82              |
| 12:AB:54:TYR:HE2   | 14:AE:291:ILE:HG23 | 1.44                     | 0.82              |
| 12:AB:152:HIS:HB3  | 12:AB:154:VAL:HG12 | 1.62                     | 0.82              |
| 20:G:105:LYS:O     | 20:G:109:GLN:NE2   | 2.12                     | 0.82              |
| 40:a:2298:A:OP1    | 53:n:72:LYS:NZ     | 2.11                     | 0.82              |
| 59:t:7:MET:HG3     | 59:t:18:ARG:CZ     | 2.10                     | 0.82              |
| 9:9:48:ALA:HB3     | 9:9:51:TYR:CE1     | 2.09                     | 0.82              |
| 12:AB:146:ILE:HD11 | 29:P:88:MET:CA     | 2.09                     | 0.82              |
| 9:9:3:LEU:HD11     | 9:9:5:LEU:HD23     | 1.62                     | 0.82              |
| 10:B:6:G:O2'       | 10:B:7:G:O5'       | 1.96                     | 0.82              |
| 55:p:104:ASN:ND2   | 55:p:114:ASP:OD1   | 2.12                     | 0.82              |
| 14:AE:78:LEU:C     | 14:AE:81:ARG:NH1   | 2.24                     | 0.82              |
| 53:n:73:SER:OG     | 53:n:79:ILE:O      | 1.96                     | 0.82              |
| 6:5:9:DG:H5''      | 11:AA:473:ARG:CG   | 1.95                     | 0.82              |
| 14:AE:81:ARG:H     | 14:AE:81:ARG:HD2   | 1.45                     | 0.82              |
| 55:p:7:ALA:O       | 55:p:69:ARG:NE     | 2.12                     | 0.82              |
| 9:9:129:LEU:H      | 9:9:130:PRO:HD2    | 1.45                     | 0.81              |
| 10:A:6:G:O2'       | 10:A:7:G:O5'       | 1.96                     | 0.81              |
| 6:5:10:DT:C5       | 11:AA:62:TYR:HD2   | 1.81                     | 0.81              |
| 6:5:11:DA:C4'      | 12:AB:67:THR:HG22  | 2.10                     | 0.81              |
| 9:9:1:MET:HE1      | 9:9:7:ASP:HB3      | 1.61                     | 0.81              |
| 40:a:1613:G:O2'    | 52:m:3:ARG:NH2     | 2.12                     | 0.81              |
| 59:t:12:ASP:OD2    | 59:t:85:VAL:HG13   | 1.80                     | 0.81              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:5:10:DT:C4      | 11:AA:62:TYR:CD2   | 2.68                     | 0.81              |
| 40:a:2356:U:O3'   | 41:b:20:ARG:NH1    | 2.14                     | 0.81              |
| 11:AA:387:ASN:CB  | 11:AA:394:ARG:HH11 | 1.93                     | 0.81              |
| 38:Y:14:ALA:HB3   | 38:Y:51:GLY:H      | 1.45                     | 0.81              |
| 38:Y:45:THR:HG22  | 38:Y:50:LYS:HD3    | 1.59                     | 0.81              |
| 17:D:311:C:OP1    | 34:U:31:ARG:NH2    | 2.13                     | 0.81              |
| 38:Y:58:ILE:HG22  | 38:Y:60:VAL:HG23   | 1.62                     | 0.81              |
| 9:9:52:MET:HG2    | 9:9:95:LEU:HD11    | 1.62                     | 0.81              |
| 65:z:69:ALA:HB1   | 65:z:74:ILE:HG23   | 1.63                     | 0.81              |
| 9:9:25:ALA:HB3    | 9:9:99:PHE:CD2     | 2.16                     | 0.81              |
| 12:AB:141:LEU:HA  | 12:AB:152:HIS:C    | 2.06                     | 0.81              |
| 17:D:107:G:O6     | 18:E:10:ARG:NE     | 2.13                     | 0.81              |
| 18:E:28:MET:HE1   | 18:E:58:VAL:HA     | 1.64                     | 0.80              |
| 40:a:2682:A:C8    | 49:j:11:MET:CE     | 2.65                     | 0.80              |
| 51:l:1:MET:HE1    | 51:l:20:GLY:CA     | 2.11                     | 0.80              |
| 51:l:112:LEU:HD12 | 51:l:117:ARG:HB2   | 1.62                     | 0.80              |
| 65:z:74:ILE:HD13  | 65:z:79:PHE:HD1    | 1.47                     | 0.80              |
| 60:u:122:VAL:HG13 | 60:u:125:LEU:HD11  | 1.61                     | 0.80              |
| 11:AA:377:THR:OG1 | 12:AB:62:GLU:CA    | 2.30                     | 0.80              |
| 40:a:1818:U:O5'   | 47:h:156:ARG:NH2   | 2.14                     | 0.80              |
| 1:0:86:GLN:OE1    | 40:a:1225:G:H4'    | 1.81                     | 0.80              |
| 38:Y:40:ALA:HB1   | 38:Y:68:PHE:CE1    | 2.16                     | 0.80              |
| 9:9:46:ARG:HG3    | 9:9:94:ARG:NH2     | 1.94                     | 0.80              |
| 40:a:2393:U:H5''  | 54:o:30:ARG:NH1    | 1.97                     | 0.80              |
| 8:7:20:U:OP2      | 22:I:74:GLY:HA3    | 1.82                     | 0.80              |
| 38:Y:81:LYS:HZ2   | 38:Y:86:LYS:HE2    | 1.46                     | 0.80              |
| 8:7:2:U:OP1       | 17:D:1505:G:C8     | 2.33                     | 0.80              |
| 12:AB:54:TYR:CE2  | 14:AE:291:ILE:CG2  | 2.65                     | 0.80              |
| 12:AB:148:LYS:HZ1 | 29:P:102:LEU:CD2   | 1.95                     | 0.80              |
| 19:F:37:PHE:HB2   | 30:Q:126:LYS:CE    | 2.10                     | 0.80              |
| 41:b:28:GLY:O     | 41:b:66:LYS:NZ     | 2.13                     | 0.80              |
| 59:t:98:ARG:NH2   | 59:t:118:LEU:O     | 2.14                     | 0.80              |
| 40:a:2636:C:H4'   | 49:j:81:GLU:OE1    | 1.82                     | 0.80              |
| 12:AB:140:MET:CA  | 12:AB:152:HIS:O    | 2.29                     | 0.79              |
| 40:a:1655:A:H1'   | 49:j:118:PHE:HE2   | 1.45                     | 0.79              |
| 4:3:46:GLN:OE1    | 4:3:56:GLY:HA2     | 1.81                     | 0.79              |
| 40:a:2393:U:P     | 54:o:30:ARG:HE     | 2.04                     | 0.79              |
| 7:6:23:DC:H5'     | 14:AE:259:ARG:HH12 | 1.43                     | 0.79              |
| 47:h:258:ARG:NH1  | 47:h:264:ASP:OD1   | 2.14                     | 0.79              |
| 53:n:117:LEU:HD13 | 53:n:176:PRO:HG2   | 1.64                     | 0.79              |
| 17:D:275:G:H4'    | 35:V:16:LYS:HD2    | 1.64                     | 0.79              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:l:111:GLU:OE2   | 51:l:114:ARG:NH1  | 2.14                     | 0.79              |
| 59:t:20:MET:HB3    | 59:t:44:LYS:NZ    | 1.98                     | 0.79              |
| 9:9:112:ALA:O      | 9:9:123:ILE:HD11  | 1.83                     | 0.79              |
| 38:Y:9:LYS:HE2     | 38:Y:55:PRO:HB3   | 1.63                     | 0.79              |
| 6:5:10:DT:C2       | 12:AB:71:ALA:CB   | 2.61                     | 0.79              |
| 7:6:25:DT:H3'      | 11:AA:496:LYS:CG  | 2.13                     | 0.79              |
| 12:AB:146:ILE:HD11 | 29:P:88:MET:CG    | 2.12                     | 0.79              |
| 26:M:20:SER:HB3    | 26:M:23:LEU:HD13  | 1.63                     | 0.79              |
| 47:h:53:HIS:HE2    | 47:h:219:THR:HA   | 1.45                     | 0.79              |
| 25:L:70:VAL:O      | 25:L:74:LEU:HD23  | 1.81                     | 0.79              |
| 38:Y:102:ARG:HD2   | 38:Y:141:ASP:CA   | 2.13                     | 0.79              |
| 47:h:130:LEU:HA    | 47:h:189:ARG:HH11 | 1.46                     | 0.79              |
| 2:1:98:LYS:HD2     | 40:a:2012:G:OP1   | 1.83                     | 0.79              |
| 9:9:3:LEU:CD1      | 9:9:4:ASN:H       | 1.96                     | 0.79              |
| 48:i:46:ASP:OD2    | 48:i:53:LYS:NZ    | 2.15                     | 0.79              |
| 9:9:5:LEU:O        | 9:9:9:GLN:NE2     | 2.15                     | 0.79              |
| 9:9:77:VAL:HG13    | 9:9:114:GLU:OE1   | 1.81                     | 0.79              |
| 8:7:3:G:C5'        | 17:D:1500:A:N6    | 2.46                     | 0.79              |
| 17:D:673:A:H2'     | 17:D:674:G:C8     | 2.18                     | 0.79              |
| 32:S:12:LYS:O      | 32:S:16:LEU:HD23  | 1.83                     | 0.79              |
| 40:a:1453:A:N1     | 62:w:74:GLU:OE1   | 2.16                     | 0.79              |
| 28:O:56:ASP:O      | 28:O:60:LYS:NZ    | 2.16                     | 0.78              |
| 40:a:1276:A:O2'    | 62:w:20:MET:CE    | 2.30                     | 0.78              |
| 9:9:118:ILE:HB     | 9:9:119:PRO:HD3   | 1.64                     | 0.78              |
| 27:N:9:ASP:OD2     | 27:N:13:ARG:NH1   | 2.15                     | 0.78              |
| 27:N:27:MET:N      | 27:N:58:GLU:OE2   | 2.16                     | 0.78              |
| 42:c:30:LEU:HD12   | 42:c:31:PRO:HD2   | 1.63                     | 0.78              |
| 55:p:107:LEU:HB3   | 55:p:152:ARG:HE   | 1.47                     | 0.78              |
| 6:5:10:DT:C2'      | 12:AB:71:ALA:H    | 1.95                     | 0.78              |
| 46:g:18:CYS:HB3    | 46:g:40:CYS:CB    | 2.13                     | 0.78              |
| 53:n:142:ASP:HB3   | 53:n:145:LYS:HE2  | 1.65                     | 0.78              |
| 63:x:104:GLN:NE2   | 63:x:108:ASP:OD2  | 2.16                     | 0.78              |
| 21:H:306:VAL:HA    | 21:H:309:MET:SD   | 2.23                     | 0.78              |
| 12:AB:51:PHE:CZ    | 14:AE:288:PRO:CD  | 2.66                     | 0.78              |
| 16:C:60:LYS:HZ3    | 17:D:735:C:P      | 2.05                     | 0.78              |
| 23:J:62:ARG:NH1    | 23:J:69:GLU:OE2   | 2.16                     | 0.78              |
| 26:M:40:GLU:OE2    | 28:O:41:ARG:NH2   | 2.17                     | 0.78              |
| 38:Y:9:LYS:HE2     | 38:Y:55:PRO:CG    | 2.14                     | 0.78              |
| 6:5:10:DT:C2       | 12:AB:71:ALA:HB3  | 1.84                     | 0.78              |
| 16:C:38:LYS:HE2    | 16:C:38:LYS:HA    | 1.64                     | 0.78              |
| 9:9:34:THR:O       | 9:9:38:MET:HG2    | 1.83                     | 0.78              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:9:60:LEU:HD23   | 9:9:64:VAL:HG21    | 1.65                     | 0.78              |
| 9:9:81:LEU:HD21   | 40:a:1107:G:H4'    | 1.64                     | 0.78              |
| 34:U:3:THR:HG21   | 34:U:5:ARG:CZ      | 2.14                     | 0.78              |
| 56:q:2:LYS:NZ     | 56:q:32:LYS:O      | 2.17                     | 0.78              |
| 12:AB:110:PRO:HG3 | 12:AB:116:VAL:HG11 | 1.65                     | 0.77              |
| 36:W:40:ILE:HG23  | 36:W:44:MET:SD     | 2.24                     | 0.77              |
| 9:9:94:ARG:HB2    | 9:9:97:LYS:HE2     | 1.67                     | 0.77              |
| 26:M:18:PHE:HE2   | 26:M:47:LEU:HD21   | 1.48                     | 0.77              |
| 59:t:8:LEU:C      | 59:t:18:ARG:HH12   | 1.92                     | 0.77              |
| 10:B:18:G:N2      | 10:B:55:U:O2       | 2.17                     | 0.77              |
| 34:U:3:THR:HG21   | 34:U:5:ARG:NH1     | 1.99                     | 0.77              |
| 12:AB:146:ILE:CD1 | 29:P:88:MET:HG3    | 2.15                     | 0.77              |
| 16:C:60:LYS:HZ2   | 17:D:734:G:H2'     | 1.49                     | 0.77              |
| 17:D:1227:A:OP1   | 37:X:93:ARG:NH2    | 2.18                     | 0.77              |
| 38:Y:93:ASN:C     | 38:Y:94:LYS:HD2    | 2.10                     | 0.77              |
| 40:a:1801:A:P     | 47:h:146:MET:HE1   | 2.25                     | 0.77              |
| 17:D:375:U:OP2    | 34:U:70:ARG:NH2    | 2.17                     | 0.77              |
| 17:D:652:U:O3'    | 27:N:56:LYS:NZ     | 2.13                     | 0.77              |
| 9:9:19:ALA:HA     | 9:9:70:GLU:HG2     | 1.66                     | 0.77              |
| 39:Z:2:ILE:HG22   | 39:Z:4:LYS:H       | 1.50                     | 0.77              |
| 17:D:375:U:P      | 34:U:70:ARG:HE     | 2.07                     | 0.77              |
| 30:Q:84:VAL:HG23  | 30:Q:107:ILE:HD11  | 1.67                     | 0.77              |
| 30:Q:87:LYS:CG    | 30:Q:113:VAL:HG23  | 2.15                     | 0.76              |
| 40:a:1405:U:H2'   | 40:a:1406:U:C6     | 2.20                     | 0.76              |
| 40:a:2511:U:C4'   | 49:j:130:GLN:OE1   | 2.33                     | 0.76              |
| 12:AB:146:ILE:CD1 | 29:P:88:MET:HA     | 2.14                     | 0.76              |
| 58:s:37:ARG:HA    | 58:s:118:MET:CE    | 2.14                     | 0.76              |
| 39:Z:14:MET:HG3   | 39:Z:15:SER:H      | 1.49                     | 0.76              |
| 40:a:1828:G:O6    | 47:h:221:ARG:NH1   | 2.19                     | 0.76              |
| 40:a:2335:A:OP2   | 63:x:13:ARG:CZ     | 2.34                     | 0.76              |
| 62:w:12:ARG:O     | 62:w:17:ARG:NH2    | 2.19                     | 0.76              |
| 6:5:11:DA:C4'     | 12:AB:67:THR:CG2   | 2.64                     | 0.76              |
| 8:7:2:U:OP1       | 17:D:1505:G:H8     | 1.65                     | 0.76              |
| 61:v:1:MET:HA     | 61:v:1:MET:HE3     | 1.67                     | 0.76              |
| 9:9:27:VAL:HG13   | 9:9:83:ALA:HB3     | 1.66                     | 0.76              |
| 12:AB:139:SER:O   | 12:AB:153:SER:HA   | 1.85                     | 0.76              |
| 12:AB:152:HIS:HB3 | 12:AB:154:VAL:CG1  | 2.15                     | 0.76              |
| 36:W:44:MET:SD    | 36:W:62:VAL:HG11   | 2.25                     | 0.76              |
| 12:AB:9:CYS:H     | 12:AB:53:ASN:HB3   | 1.48                     | 0.76              |
| 20:G:49:MET:CE    | 20:G:201:PRO:HD3   | 2.16                     | 0.76              |
| 40:a:686:U:O4     | 52:m:12:ARG:HD3    | 1.86                     | 0.76              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 40:a:1406:U:O2'  | 40:a:1407:G:O5'   | 2.02                     | 0.76              |
| 9:9:43:LYS:HZ2   | 9:9:98:GLU:HB2    | 1.49                     | 0.76              |
| 40:a:2314:A:OP1  | 53:n:88:LYS:NZ    | 2.18                     | 0.76              |
| 58:s:15:TRP:CZ3  | 58:s:135:GLN:HA   | 2.21                     | 0.76              |
| 6:5:10:DT:C5     | 11:AA:62:TYR:HE2  | 1.97                     | 0.76              |
| 10:A:18:G:N2     | 10:A:55:U:O2      | 2.17                     | 0.76              |
| 12:AB:51:PHE:CE2 | 14:AE:288:PRO:HG2 | 2.06                     | 0.76              |
| 59:t:20:MET:HB3  | 59:t:44:LYS:HZ3   | 1.48                     | 0.76              |
| 40:a:196:A:OP2   | 60:u:47:ARG:NH1   | 2.18                     | 0.76              |
| 9:9:5:LEU:C      | 9:9:9:GLN:HE22    | 1.94                     | 0.75              |
| 23:J:58:LYS:NZ   | 23:J:69:GLU:OE2   | 2.15                     | 0.75              |
| 53:n:4:LEU:HD11  | 53:n:101:GLU:CA   | 2.16                     | 0.75              |
| 2:1:11:ARG:CZ    | 2:1:98:LYS:HE3    | 2.15                     | 0.75              |
| 9:9:134:GLU:OE2  | 9:9:136:ILE:HG22  | 1.85                     | 0.75              |
| 20:G:30:PHE:CD1  | 20:G:201:PRO:HG3  | 2.21                     | 0.75              |
| 9:9:77:VAL:HG12  | 9:9:82:ILE:HG21   | 1.68                     | 0.75              |
| 12:AB:141:LEU:O  | 12:AB:151:LYS:CA  | 2.34                     | 0.75              |
| 21:H:52:GLN:OE1  | 21:H:86:ARG:CB    | 2.34                     | 0.75              |
| 25:L:42:TRP:HZ3  | 25:L:45:ARG:HH22  | 1.32                     | 0.75              |
| 40:a:742:A:H2'   | 40:a:743:A:C8     | 2.22                     | 0.75              |
| 40:a:2297:A:N1   | 40:a:2321:U:C4    | 2.53                     | 0.75              |
| 64:y:71:GLU:OE1  | 64:y:101:ARG:NE   | 2.19                     | 0.75              |
| 2:1:24:ILE:HG21  | 2:1:36:LEU:HD11   | 1.68                     | 0.75              |
| 9:9:37:LYS:O     | 9:9:41:LEU:HG     | 1.86                     | 0.75              |
| 20:G:20:THR:HA   | 20:G:39:HIS:CE1   | 2.21                     | 0.75              |
| 5:4:50:MET:O     | 5:4:56:PHE:CE2    | 2.38                     | 0.75              |
| 17:D:550:G:O2'   | 31:R:116:LYS:NZ   | 2.18                     | 0.75              |
| 20:G:154:MET:CE  | 20:G:158:PRO:HD3  | 2.16                     | 0.75              |
| 24:K:142:ASP:O   | 24:K:145:GLU:HG3  | 1.86                     | 0.75              |
| 49:j:46:ARG:NH2  | 49:j:88:GLU:O     | 2.19                     | 0.75              |
| 12:AB:18:GLN:HG3 | 12:AB:21:LEU:HD12 | 1.69                     | 0.75              |
| 16:C:38:LYS:HD3  | 17:D:719:C:H1'    | 1.67                     | 0.75              |
| 19:F:63:GLU:OE1  | 19:F:67:ARG:NH1   | 2.20                     | 0.75              |
| 26:M:18:PHE:CE2  | 26:M:47:LEU:HD21  | 2.21                     | 0.75              |
| 37:X:57:ARG:NH2  | 46:g:35:ASP:OD1   | 2.19                     | 0.75              |
| 38:Y:126:ARG:NH2 | 40:a:1083:U:OP1   | 2.19                     | 0.75              |
| 14:AE:59:ALA:HB1 | 14:AE:71:LEU:CD2  | 2.16                     | 0.75              |
| 30:Q:87:LYS:HG2  | 30:Q:113:VAL:HG23 | 1.67                     | 0.75              |
| 37:X:28:THR:HG23 | 37:X:31:LYS:HE3   | 1.68                     | 0.75              |
| 40:a:537:G:OP2   | 58:s:2:LYS:NZ     | 2.20                     | 0.75              |
| 53:n:56:ASP:OD2  | 53:n:150:ARG:NH1  | 2.20                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:5:10:DT:H2''     | 12:AB:69:ILE:C     | 2.11                     | 0.74              |
| 17:D:1217:C:OP2    | 32:S:9:ARG:NH2     | 2.19                     | 0.74              |
| 33:T:64:ARG:CZ     | 33:T:89:ARG:HH22   | 2.00                     | 0.74              |
| 40:a:1276:A:O2'    | 62:w:20:MET:HE2    | 1.87                     | 0.74              |
| 51:l:90:GLN:NE2    | 51:l:91:ASP:O      | 2.20                     | 0.74              |
| 2:1:25:ARG:HH22    | 40:a:520:G:P       | 2.10                     | 0.74              |
| 58:s:15:TRP:HZ3    | 58:s:135:GLN:HA    | 1.50                     | 0.74              |
| 9:9:59:LEU:HD13    | 9:9:62:ARG:HD2     | 1.70                     | 0.74              |
| 41:b:68:LYS:NZ     | 41:b:70:GLU:OE1    | 2.19                     | 0.74              |
| 43:d:42:C:O5'      | 53:n:64:LYS:NZ     | 2.20                     | 0.74              |
| 6:5:10:DT:C4       | 11:AA:62:TYR:CE2   | 2.74                     | 0.74              |
| 17:D:739:C:O2'     | 33:T:42:HIS:ND1    | 2.18                     | 0.74              |
| 57:r:6:LEU:HD11    | 57:r:37:VAL:HG23   | 1.69                     | 0.74              |
| 12:AB:89:PRO:HD2   | 14:AE:290:ILE:HG21 | 1.68                     | 0.74              |
| 16:C:60:LYS:NZ     | 17:D:734:G:O3'     | 2.20                     | 0.74              |
| 59:t:42:THR:O      | 59:t:44:LYS:NZ     | 2.19                     | 0.74              |
| 5:4:57:TYR:HB3     | 61:v:136:MET:CE    | 2.16                     | 0.74              |
| 9:9:59:LEU:HD22    | 9:9:62:ARG:NE      | 2.02                     | 0.74              |
| 23:J:105:MET:CE    | 23:J:171:LEU:HD13  | 2.18                     | 0.74              |
| 12:AB:147:ASN:ND2  | 29:P:100:ILE:CG1   | 2.36                     | 0.74              |
| 21:H:36:VAL:O      | 21:H:37:LEU:HD12   | 1.87                     | 0.74              |
| 9:9:36:ASP:O       | 9:9:39:THR:HG22    | 1.87                     | 0.74              |
| 14:AE:74:LYS:HZ3   | 29:P:89:ARG:CB     | 2.00                     | 0.74              |
| 21:H:303:LEU:O     | 21:H:305:HIS:N     | 2.20                     | 0.74              |
| 5:4:45:ASP:OD1     | 5:4:46:LYS:N       | 2.21                     | 0.74              |
| 17:D:404:G:OP1     | 23:J:115:ARG:NH1   | 2.19                     | 0.74              |
| 38:Y:56:VAL:CA     | 38:Y:71:LYS:HZ1    | 2.00                     | 0.74              |
| 9:9:23:LEU:HD11    | 9:9:96:PHE:CD2     | 2.23                     | 0.73              |
| 18:E:21:ASN:C      | 18:E:25:ARG:HE     | 1.96                     | 0.73              |
| 55:p:69:ARG:NH1    | 55:p:73:ASN:OD1    | 2.21                     | 0.73              |
| 2:1:25:ARG:NH2     | 40:a:520:G:H5'     | 2.03                     | 0.73              |
| 11:AA:377:THR:CG2  | 12:AB:62:GLU:HB3   | 2.18                     | 0.73              |
| 12:AB:145:LEU:HD23 | 29:P:88:MET:SD     | 2.28                     | 0.73              |
| 62:w:33:ILE:HD11   | 62:w:112:TYR:CD1   | 2.23                     | 0.73              |
| 62:w:60:VAL:HG22   | 62:w:63:ARG:NH1    | 2.03                     | 0.73              |
| 5:4:75:GLN:HG3     | 5:4:92:VAL:HG23    | 1.70                     | 0.73              |
| 6:5:10:DT:N3       | 12:AB:72:THR:OG1   | 2.21                     | 0.73              |
| 12:AB:21:LEU:HB3   | 12:AB:26:VAL:HG11  | 1.70                     | 0.73              |
| 12:AB:148:LYS:HZ1  | 29:P:102:LEU:HD23  | 1.51                     | 0.73              |
| 17:D:376:G:H5''    | 34:U:5:ARG:HD2     | 1.67                     | 0.73              |
| 17:D:1158:C:O2'    | 20:G:132:LYS:NZ    | 2.21                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:Y:9:LYS:HE2    | 38:Y:55:PRO:CB     | 2.17                     | 0.73              |
| 38:Y:102:ARG:CD   | 38:Y:141:ASP:HA    | 2.18                     | 0.73              |
| 39:Z:6:GLN:OE1    | 39:Z:10:ALA:HB2    | 1.88                     | 0.73              |
| 41:b:21:LEU:HD21  | 41:b:41:ARG:HE     | 1.51                     | 0.73              |
| 14:AE:81:ARG:HD2  | 14:AE:81:ARG:N     | 2.03                     | 0.73              |
| 23:J:100:ASN:OD1  | 23:J:111:ARG:NH1   | 2.21                     | 0.73              |
| 61:v:97:GLN:N     | 61:v:100:LYS:HE3   | 2.03                     | 0.73              |
| 9:9:129:LEU:HD12  | 9:9:130:PRO:HD3    | 1.70                     | 0.73              |
| 16:C:38:LYS:NZ    | 17:D:718:A:C2      | 2.57                     | 0.73              |
| 17:D:375:U:OP1    | 34:U:70:ARG:HG2    | 1.88                     | 0.73              |
| 33:T:76:ALA:O     | 33:T:80:GLN:NE2    | 2.22                     | 0.73              |
| 38:Y:100:ILE:HG13 | 38:Y:139:VAL:CG2   | 2.18                     | 0.73              |
| 48:i:55:ILE:HD13  | 62:w:112:TYR:CZ    | 2.23                     | 0.73              |
| 8:7:13:U:H3       | 23:J:47:ARG:HH11   | 1.37                     | 0.73              |
| 9:9:43:LYS:NZ     | 9:9:98:GLU:HB2     | 2.04                     | 0.73              |
| 9:9:56:ARG:O      | 9:9:56:ARG:HG2     | 1.88                     | 0.73              |
| 12:AB:89:PRO:CD   | 14:AE:290:ILE:HG21 | 2.18                     | 0.73              |
| 40:a:465:G:OP1    | 52:m:12:ARG:NH2    | 2.22                     | 0.73              |
| 59:t:17:ARG:HB2   | 59:t:45:GLU:OE1    | 1.88                     | 0.73              |
| 31:R:56:ARG:HG2   | 31:R:62:GLU:OE2    | 1.89                     | 0.73              |
| 46:g:18:CYS:CB    | 46:g:40:CYS:HB3    | 2.17                     | 0.73              |
| 28:O:47:VAL:HA    | 28:O:50:GLN:HG2    | 1.70                     | 0.73              |
| 22:I:142:MET:HE3  | 22:I:170:GLU:OE1   | 1.89                     | 0.73              |
| 25:L:36:ILE:CD1   | 25:L:64:VAL:HG22   | 2.19                     | 0.73              |
| 26:M:103:TRP:CG   | 26:M:137:LYS:HZ2   | 2.07                     | 0.73              |
| 40:a:1278:C:H4'   | 62:w:24:MET:HE1    | 1.70                     | 0.73              |
| 47:h:130:LEU:HA   | 47:h:189:ARG:NH1   | 2.03                     | 0.73              |
| 9:9:78:GLY:N      | 9:9:79:PRO:HD2     | 2.04                     | 0.73              |
| 16:C:73:ARG:NH1   | 30:Q:113:VAL:HG12  | 2.02                     | 0.73              |
| 42:c:71:LEU:HB3   | 42:c:76:GLU:OE2    | 1.88                     | 0.73              |
| 46:g:18:CYS:CB    | 46:g:40:CYS:CB     | 2.67                     | 0.72              |
| 54:o:25:LYS:HB3   | 60:u:62:PRO:HG2    | 1.71                     | 0.72              |
| 17:D:13:U:C4      | 17:D:915:A:N6      | 2.57                     | 0.72              |
| 33:T:21:ASP:O     | 33:T:22:THR:OG1    | 2.07                     | 0.72              |
| 2:1:23:LEU:HD11   | 48:i:24:ALA:HB2    | 1.70                     | 0.72              |
| 9:9:94:ARG:HB3    | 9:9:97:LYS:HZ3     | 1.54                     | 0.72              |
| 16:C:18:VAL:O     | 16:C:51:TYR:OH     | 2.06                     | 0.72              |
| 38:Y:100:ILE:HD11 | 38:Y:139:VAL:HB    | 1.69                     | 0.72              |
| 38:Y:102:ARG:CZ   | 38:Y:139:VAL:HG11  | 2.19                     | 0.72              |
| 11:AA:387:ASN:OD1 | 11:AA:394:ARG:NH1  | 2.21                     | 0.72              |
| 10:B:76:A:C2      | 40:a:2493:U:H4'    | 2.24                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:I:147:LYS:NZ    | 22:I:204:LYS:O     | 2.22                     | 0.72              |
| 61:v:50:ARG:HA     | 61:v:53:MET:SD     | 2.29                     | 0.72              |
| 61:v:73:ILE:HD11   | 61:v:93:VAL:HG22   | 1.70                     | 0.72              |
| 17:D:311:C:P       | 34:U:31:ARG:HH22   | 2.13                     | 0.72              |
| 17:D:973:G:O4'     | 29:P:57:VAL:HG22   | 1.90                     | 0.72              |
| 38:Y:14:ALA:CB     | 38:Y:50:LYS:HD2    | 2.16                     | 0.72              |
| 40:a:2884:U:OP2    | 48:i:40:ARG:NH2    | 2.23                     | 0.72              |
| 53:n:127:ASN:OD1   | 53:n:158:THR:N     | 2.18                     | 0.72              |
| 55:p:85:LYS:HE3    | 55:p:164:TYR:CD1   | 2.24                     | 0.72              |
| 5:4:77:VAL:CG2     | 5:4:79:ARG:HE      | 2.03                     | 0.72              |
| 10:A:53:G:C2       | 10:A:54:U:C5       | 2.77                     | 0.72              |
| 23:J:184:ARG:NH1   | 23:J:187:GLU:OE1   | 2.22                     | 0.72              |
| 14:AE:59:ALA:HB1   | 14:AE:71:LEU:HD22  | 1.71                     | 0.72              |
| 14:AE:64:PRO:HG3   | 14:AE:90:VAL:CG1   | 2.20                     | 0.72              |
| 19:F:32:VAL:HG12   | 19:F:36:GLU:OE1    | 1.90                     | 0.72              |
| 55:p:17:VAL:O      | 55:p:18:LYS:HE2    | 1.89                     | 0.72              |
| 12:AB:24:GLN:HB2   | 12:AB:26:VAL:HG23  | 1.71                     | 0.72              |
| 20:G:19:GLN:NE2    | 21:H:75:VAL:O      | 2.23                     | 0.72              |
| 47:h:123:ALA:HB1   | 47:h:125:LYS:NZ    | 2.04                     | 0.72              |
| 6:5:9:DG:OP2       | 11:AA:470:ARG:HA   | 1.90                     | 0.72              |
| 9:9:56:ARG:NH2     | 40:a:1084:A:O4'    | 2.23                     | 0.72              |
| 11:AA:387:ASN:CG   | 11:AA:394:ARG:HH12 | 1.81                     | 0.72              |
| 12:AB:154:VAL:HG11 | 12:AB:159:PHE:HB3  | 1.72                     | 0.72              |
| 10:B:13:C:OP2      | 40:a:1907:G:N2     | 2.23                     | 0.72              |
| 10:B:53:G:C2       | 10:B:54:U:C5       | 2.77                     | 0.72              |
| 17:D:653:U:C6      | 27:N:56:LYS:HE3    | 2.25                     | 0.72              |
| 18:E:75:HIS:CE1    | 18:E:79:LEU:HD11   | 2.25                     | 0.72              |
| 26:M:55:GLY:O      | 26:M:56:LYS:O      | 2.07                     | 0.72              |
| 29:P:47:GLU:N      | 29:P:47:GLU:OE1    | 2.23                     | 0.72              |
| 8:7:18:U:C6        | 8:7:18:U:H5''      | 2.24                     | 0.72              |
| 14:AE:77:ARG:NE    | 14:AE:77:ARG:HA    | 2.04                     | 0.72              |
| 17:D:13:U:O4       | 17:D:21:G:C2       | 2.43                     | 0.72              |
| 33:T:63:ARG:O      | 33:T:67:LEU:HD23   | 1.90                     | 0.72              |
| 37:X:81:MET:HE2    | 40:a:888:C:C6      | 2.24                     | 0.72              |
| 17:D:636:U:H4'     | 35:V:6:ARG:CZ      | 2.19                     | 0.71              |
| 38:Y:81:LYS:HD2    | 38:Y:81:LYS:N      | 2.05                     | 0.71              |
| 17:D:1328:C:O2'    | 37:X:29:ARG:NH2    | 2.23                     | 0.71              |
| 19:F:13:ASP:OD1    | 19:F:14:VAL:N      | 2.22                     | 0.71              |
| 22:I:39:VAL:O      | 22:I:43:LEU:HD23   | 1.90                     | 0.71              |
| 22:I:166:GLU:OE1   | 22:I:166:GLU:N     | 2.23                     | 0.71              |
| 23:J:76:TYR:CE2    | 23:J:204:TYR:HB2   | 2.24                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:a:987:C:O3'    | 45:f:11:ARG:NH1   | 2.23                     | 0.71              |
| 29:P:18:ILE:O     | 29:P:22:THR:HG23  | 1.90                     | 0.71              |
| 1:0:10:LYS:HE2    | 40:a:994:C:O2'    | 1.90                     | 0.71              |
| 9:9:47:GLU:HB3    | 9:9:51:TYR:CZ     | 2.24                     | 0.71              |
| 12:AB:141:LEU:N   | 12:AB:153:SER:HB3 | 2.05                     | 0.71              |
| 14:AE:68:TYR:HA   | 14:AE:92:VAL:HG23 | 1.72                     | 0.71              |
| 14:AE:85:CYS:SG   | 67:AE:1502:ZN:ZN  | 1.79                     | 0.71              |
| 22:I:142:MET:HE1  | 22:I:148:GLY:HA2  | 1.72                     | 0.71              |
| 40:a:2469:A:N6    | 40:a:2481:G:O2'   | 2.23                     | 0.71              |
| 8:7:3:G:H5''      | 17:D:1500:A:H62   | 1.49                     | 0.71              |
| 17:D:1208:C:H2'   | 17:D:1209:C:H6    | 1.56                     | 0.71              |
| 40:a:1824:G:OP1   | 47:h:52:ARG:NH2   | 2.23                     | 0.71              |
| 40:a:2328:A:H2'   | 40:a:2329:U:C6    | 2.25                     | 0.71              |
| 46:g:5:ILE:HD12   | 53:n:64:LYS:HE3   | 1.72                     | 0.71              |
| 51:l:6:LYS:NZ     | 51:l:120:VAL:O    | 2.24                     | 0.71              |
| 59:t:8:LEU:C      | 59:t:18:ARG:NH1   | 2.49                     | 0.71              |
| 8:7:11:U:O2'      | 24:K:33:PHE:HE1   | 1.70                     | 0.71              |
| 9:9:122:GLN:HG2   | 9:9:123:ILE:N     | 2.06                     | 0.71              |
| 24:K:69:ARG:CZ    | 24:K:69:ARG:HA    | 2.20                     | 0.71              |
| 33:T:64:ARG:NH1   | 33:T:64:ARG:HA    | 2.05                     | 0.71              |
| 65:z:92:ARG:HG3   | 65:z:95:LEU:HD12  | 1.71                     | 0.71              |
| 2:1:86:MET:HE1    | 2:1:88:ARG:HD3    | 1.70                     | 0.71              |
| 31:R:5:ASN:OD1    | 35:V:36:LYS:NZ    | 2.24                     | 0.71              |
| 2:1:83:LYS:HB2    | 2:1:95:ARG:HD3    | 1.72                     | 0.71              |
| 17:D:375:U:OP1    | 34:U:70:ARG:NE    | 2.24                     | 0.71              |
| 22:I:74:GLY:O     | 22:I:78:GLY:N     | 2.24                     | 0.71              |
| 32:S:90:ARG:HG3   | 32:S:92:GLU:CD    | 2.15                     | 0.71              |
| 51:l:6:LYS:NZ     | 51:l:120:VAL:N    | 2.39                     | 0.71              |
| 9:9:27:VAL:CG1    | 9:9:83:ALA:HB3    | 2.20                     | 0.71              |
| 9:9:31:ARG:HD2    | 40:a:1053:C:HO2'  | 1.53                     | 0.71              |
| 12:AB:123:PHE:HE1 | 29:P:85:ASP:HB3   | 1.43                     | 0.71              |
| 40:a:871:U:H2'    | 40:a:872:U:C6     | 2.26                     | 0.71              |
| 11:AA:377:THR:OG1 | 12:AB:62:GLU:CG   | 2.38                     | 0.71              |
| 17:D:564:C:P      | 31:R:12:ARG:NH2   | 2.64                     | 0.71              |
| 28:O:112:GLU:OE2  | 28:O:115:LYS:NZ   | 2.23                     | 0.71              |
| 30:Q:72:ASP:O     | 30:Q:75:LYS:NZ    | 2.21                     | 0.71              |
| 40:a:1825:U:OP2   | 47:h:52:ARG:NH1   | 2.23                     | 0.71              |
| 58:s:15:TRP:CZ3   | 58:s:135:GLN:HG3  | 2.25                     | 0.71              |
| 9:9:6:GLN:HA      | 9:9:9:GLN:NE2     | 2.06                     | 0.70              |
| 21:H:332:VAL:HG22 | 21:H:342:ILE:HD11 | 1.72                     | 0.70              |
| 62:w:42:LYS:N     | 62:w:42:LYS:HD3   | 2.05                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:46:GLN:NE2    | 4:3:47:LYS:O      | 2.24                     | 0.70              |
| 12:AB:141:LEU:H   | 12:AB:153:SER:HB3 | 1.56                     | 0.70              |
| 24:K:93:ARG:HB3   | 24:K:93:ARG:CZ    | 2.21                     | 0.70              |
| 40:a:2780:G:P     | 58:s:120:ARG:HH11 | 2.13                     | 0.70              |
| 28:O:7:TYR:N      | 28:O:89:GLU:OE2   | 2.24                     | 0.70              |
| 17:D:736:C:C5'    | 25:L:90:MET:HE2   | 2.21                     | 0.70              |
| 17:D:1376:U:OP2   | 26:M:25:LYS:NZ    | 2.24                     | 0.70              |
| 22:I:22:TRP:HZ3   | 22:I:24:ALA:HB2   | 1.54                     | 0.70              |
| 30:Q:52:PHE:HD2   | 30:Q:56:ARG:HG2   | 1.56                     | 0.70              |
| 38:Y:57:VAL:O     | 38:Y:69:VAL:HG22  | 1.91                     | 0.70              |
| 53:n:134:GLU:HG2  | 53:n:137:ILE:HG23 | 1.72                     | 0.70              |
| 58:s:15:TRP:NE1   | 58:s:53:TYR:HD2   | 1.90                     | 0.70              |
| 12:AB:6:LEU:HD13  | 14:AE:291:ILE:CD1 | 2.21                     | 0.70              |
| 17:D:636:U:H4'    | 35:V:6:ARG:NH2    | 2.06                     | 0.70              |
| 24:K:111:MET:O    | 24:K:115:LEU:HD23 | 1.91                     | 0.70              |
| 58:s:72:LYS:HD3   | 58:s:74:TYR:HH    | 1.57                     | 0.70              |
| 3:2:56:GLU:OE2    | 3:2:88:LYS:HA     | 1.90                     | 0.70              |
| 27:N:87:LYS:HD2   | 27:N:91:GLU:HB3   | 1.74                     | 0.70              |
| 57:r:33:GLN:OE1   | 57:r:35:LYS:NZ    | 2.24                     | 0.70              |
| 58:s:73:VAL:C     | 58:s:74:TYR:CD2   | 2.70                     | 0.70              |
| 22:I:24:ALA:HB3   | 22:I:29:PHE:CE2   | 2.27                     | 0.70              |
| 26:M:16:PRO:HB3   | 28:O:46:MET:HG3   | 1.73                     | 0.70              |
| 38:Y:19:PRO:HG2   | 38:Y:23:VAL:HG23  | 1.73                     | 0.70              |
| 40:a:1012:U:O4    | 58:s:30:THR:HG21  | 1.92                     | 0.70              |
| 2:1:25:ARG:HH22   | 40:a:520:G:C5'    | 2.04                     | 0.70              |
| 37:X:66:GLU:OE1   | 37:X:66:GLU:N     | 2.23                     | 0.70              |
| 40:a:1190:G:OP1   | 60:u:30:THR:OG1   | 2.10                     | 0.70              |
| 46:g:16:CYS:CB    | 46:g:37:CYS:HB3   | 2.21                     | 0.70              |
| 47:h:133:ARG:NE   | 47:h:187:ASP:OD2  | 2.25                     | 0.70              |
| 47:h:180:GLU:C    | 47:h:181:MET:HE2  | 2.17                     | 0.70              |
| 60:u:123:ARG:NH2  | 60:u:143:GLU:OE2  | 2.25                     | 0.70              |
| 10:B:38:A:O2'     | 17:D:790:A:OP1    | 2.09                     | 0.70              |
| 17:D:274:A:H4'    | 35:V:16:LYS:CE    | 2.22                     | 0.70              |
| 38:Y:100:ILE:HG13 | 38:Y:139:VAL:HG23 | 1.74                     | 0.70              |
| 56:q:25:VAL:HB    | 56:q:35:GLN:OE1   | 1.92                     | 0.70              |
| 61:v:53:MET:HE3   | 61:v:120:ALA:HB2  | 1.74                     | 0.70              |
| 9:9:142:THR:OG1   | 39:Z:7:ILE:HG21   | 1.90                     | 0.69              |
| 14:AE:59:ALA:HB2  | 14:AE:71:LEU:HD21 | 1.74                     | 0.69              |
| 20:G:126:PHE:O    | 20:G:127:ASP:O    | 2.10                     | 0.69              |
| 38:Y:19:PRO:O     | 38:Y:24:GLY:HA2   | 1.92                     | 0.69              |
| 38:Y:100:ILE:CG1  | 38:Y:139:VAL:HB   | 2.22                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:p:107:LEU:O     | 55:p:152:ARG:NH1   | 2.25                     | 0.69              |
| 61:v:39:GLY:N      | 61:v:96:ILE:O      | 2.22                     | 0.69              |
| 12:AB:123:PHE:CE2  | 29:P:81:GLU:O      | 2.46                     | 0.69              |
| 14:AE:1033:GLY:HA3 | 14:AE:1081:VAL:O   | 1.93                     | 0.69              |
| 62:w:45:ARG:O      | 62:w:49:GLU:OE1    | 2.10                     | 0.69              |
| 26:M:66:LEU:HG     | 26:M:70:ARG:HE     | 1.57                     | 0.69              |
| 40:a:2350:C:OP1    | 54:o:45:ARG:NH2    | 2.25                     | 0.69              |
| 51:l:17:THR:HA     | 51:l:21:ARG:HH21   | 1.57                     | 0.69              |
| 61:v:105:MET:SD    | 61:v:117:PHE:CZ    | 2.85                     | 0.69              |
| 6:5:10:DT:H73      | 11:AA:62:TYR:HD2   | 1.29                     | 0.69              |
| 10:A:37:A:O2'      | 10:A:38:A:H5'      | 1.93                     | 0.69              |
| 16:C:57:ARG:HE     | 16:C:61:ARG:HH12   | 1.37                     | 0.69              |
| 29:P:86:ALA:O      | 29:P:90:LEU:HD13   | 1.93                     | 0.69              |
| 33:T:28:GLN:O      | 33:T:32:LEU:HG     | 1.93                     | 0.69              |
| 38:Y:91:LYS:NZ     | 38:Y:97:VAL:HG21   | 2.07                     | 0.69              |
| 40:a:2682:A:C8     | 49:j:11:MET:HE2    | 2.25                     | 0.69              |
| 47:h:205:LEU:HD12  | 47:h:210:ALA:HB1   | 1.75                     | 0.69              |
| 10:A:6:G:HO2'      | 10:A:7:G:C5'       | 2.05                     | 0.69              |
| 18:E:12:ILE:O      | 18:E:15:GLU:HG3    | 1.92                     | 0.69              |
| 26:M:4:ARG:HG2     | 26:M:5:ARG:NH1     | 2.08                     | 0.69              |
| 37:X:71:ARG:CZ     | 37:X:72:GLU:HG3    | 2.22                     | 0.69              |
| 31:R:7:LEU:HD21    | 31:R:12:ARG:NH2    | 2.07                     | 0.69              |
| 38:Y:116:MET:CG    | 38:Y:124:MET:HG2   | 2.21                     | 0.69              |
| 60:u:55:MET:HE1    | 60:u:60:ARG:HG2    | 1.75                     | 0.69              |
| 5:4:63:ILE:HD11    | 5:4:91:PHE:CD2     | 2.28                     | 0.69              |
| 20:G:26:LYS:HD2    | 20:G:193:PRO:HG2   | 1.74                     | 0.69              |
| 20:G:27:MET:SD     | 20:G:30:PHE:HB2    | 2.33                     | 0.69              |
| 2:1:7:HIS:CD2      | 2:1:10:ALA:HB2     | 2.27                     | 0.69              |
| 12:AB:18:GLN:HA    | 12:AB:21:LEU:HB2   | 1.74                     | 0.69              |
| 12:AB:103:ASP:HB3  | 12:AB:105:VAL:HG23 | 1.75                     | 0.69              |
| 23:J:76:TYR:HE2    | 23:J:204:TYR:HB2   | 1.57                     | 0.69              |
| 25:L:42:TRP:CH2    | 25:L:102:MET:CG    | 2.74                     | 0.69              |
| 37:X:28:THR:HG23   | 37:X:31:LYS:CE     | 2.22                     | 0.69              |
| 38:Y:99:LYS:NZ     | 38:Y:140:GLU:OE2   | 2.26                     | 0.69              |
| 38:Y:102:ARG:HD2   | 38:Y:141:ASP:HA    | 1.75                     | 0.69              |
| 40:a:1653:G:H3'    | 62:w:2:ARG:HD2     | 1.74                     | 0.69              |
| 40:a:1655:A:H1'    | 49:j:118:PHE:CE2   | 2.28                     | 0.69              |
| 40:a:2356:U:H5''   | 41:b:20:ARG:CD     | 2.21                     | 0.69              |
| 40:a:2511:U:H4'    | 49:j:130:GLN:OE1   | 1.91                     | 0.69              |
| 46:g:5:ILE:HB      | 53:n:64:LYS:HD3    | 1.75                     | 0.69              |
| 53:n:69:LYS:HD3    | 53:n:84:PRO:HA     | 1.75                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 59:t:103:VAL:HG22 | 59:t:104:THR:H    | 1.58                     | 0.69              |
| 5:4:53:LYS:HD2    | 5:4:56:PHE:CE2    | 2.28                     | 0.69              |
| 12:AB:113:GLY:H   | 12:AB:133:PRO:HD2 | 1.58                     | 0.69              |
| 12:AB:148:LYS:NZ  | 29:P:102:LEU:CB   | 2.35                     | 0.69              |
| 18:E:45:ALA:O     | 18:E:48:GLN:HG3   | 1.93                     | 0.69              |
| 24:K:115:LEU:HD12 | 24:K:120:VAL:HG11 | 1.75                     | 0.69              |
| 39:Z:2:ILE:HG22   | 39:Z:5:ASP:H      | 1.58                     | 0.69              |
| 59:t:5:GLN:HA     | 59:t:20:MET:HE2   | 1.74                     | 0.69              |
| 2:1:25:ARG:HH22   | 40:a:520:G:H5'    | 1.58                     | 0.69              |
| 12:AB:104:ILE:O   | 12:AB:111:TYR:OH  | 2.10                     | 0.69              |
| 18:E:9:LYS:C      | 18:E:13:GLN:HE22  | 2.00                     | 0.69              |
| 32:S:20:TYR:HE2   | 32:S:52:PRO:HG2   | 1.58                     | 0.69              |
| 33:T:76:ALA:C     | 33:T:80:GLN:HE22  | 2.00                     | 0.69              |
| 40:a:2742:G:OP1   | 56:q:36:ARG:NH1   | 2.25                     | 0.69              |
| 9:9:44:ALA:HB1    | 9:9:52:MET:HB3    | 1.74                     | 0.68              |
| 17:D:1344:C:P     | 28:O:124:ARG:HH11 | 2.16                     | 0.68              |
| 25:L:35:LYS:NZ    | 25:L:36:ILE:O     | 2.26                     | 0.68              |
| 39:Z:14:MET:HB3   | 39:Z:17:MET:CG    | 2.21                     | 0.68              |
| 62:w:38:LEU:HD13  | 62:w:111:ALA:CB   | 2.24                     | 0.68              |
| 14:AE:79:LYS:CA   | 14:AE:81:ARG:NH2  | 2.41                     | 0.68              |
| 10:B:58:A:O2'     | 10:B:59:A:H3'     | 1.93                     | 0.68              |
| 17:D:1308:U:OP1   | 37:X:100:GLN:NE2  | 2.26                     | 0.68              |
| 35:V:16:LYS:HD3   | 35:V:16:LYS:C     | 2.17                     | 0.68              |
| 38:Y:118:GLY:O    | 38:Y:124:MET:HE3  | 1.92                     | 0.68              |
| 9:9:43:LYS:HA     | 9:9:46:ARG:CZ     | 2.24                     | 0.68              |
| 9:9:52:MET:HE1    | 9:9:85:SER:C      | 2.17                     | 0.68              |
| 12:AB:102:LYS:HE2 | 14:AE:285:LEU:HA  | 1.74                     | 0.68              |
| 10:B:6:G:HO2'     | 10:B:7:G:C5'      | 2.05                     | 0.68              |
| 24:K:111:MET:CE   | 24:K:125:ALA:HB1  | 2.23                     | 0.68              |
| 26:M:111:ARG:O    | 26:M:119:ARG:NH2  | 2.27                     | 0.68              |
| 7:6:20:DA:N6      | 8:7:33:G:N1       | 2.42                     | 0.68              |
| 8:7:11:U:H4'      | 24:K:20:ARG:HH21  | 1.53                     | 0.68              |
| 21:H:22:SER:N     | 21:H:69:ASP:OD2   | 2.26                     | 0.68              |
| 30:Q:80:LYS:HB3   | 30:Q:106:ARG:NH1  | 2.09                     | 0.68              |
| 53:n:56:ASP:HB3   | 53:n:150:ARG:NH2  | 2.07                     | 0.68              |
| 53:n:94:GLU:HA    | 53:n:97:TRP:HE3   | 1.58                     | 0.68              |
| 61:v:111:GLU:O    | 61:v:115:GLU:OE1  | 2.11                     | 0.68              |
| 12:AB:130:PHE:HA  | 12:AB:152:HIS:NE2 | 2.08                     | 0.68              |
| 12:AB:147:ASN:ND2 | 29:P:100:ILE:CG2  | 2.45                     | 0.68              |
| 18:E:25:ARG:CD    | 18:E:66:LEU:HD11  | 2.22                     | 0.68              |
| 25:L:9:MET:HE1    | 25:L:85:ILE:CG2   | 2.22                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:U:45:GLU:HG3  | 34:U:46:LYS:HD3   | 1.76                     | 0.68              |
| 45:f:16:ARG:NE   | 45:f:54:MET:SD    | 2.66                     | 0.68              |
| 2:1:19:LEU:HD21  | 48:i:22:LEU:HB2   | 1.75                     | 0.68              |
| 5:4:50:MET:HA    | 5:4:56:PHE:CZ     | 2.29                     | 0.68              |
| 8:7:8:U:OP2      | 17:D:1397:C:N3    | 2.26                     | 0.68              |
| 10:B:37:A:O2'    | 10:B:38:A:H5'     | 1.93                     | 0.68              |
| 32:S:42:TRP:CZ3  | 46:g:66:ILE:HG23  | 2.29                     | 0.68              |
| 37:X:90:ARG:CD   | 37:X:97:VAL:HA    | 2.23                     | 0.68              |
| 61:v:1:MET:HE1   | 61:v:43:ALA:C     | 2.18                     | 0.68              |
| 4:3:72:ILE:HD12  | 4:3:83:VAL:HG21   | 1.76                     | 0.68              |
| 18:E:78:ASN:O    | 18:E:82:GLN:OE1   | 2.10                     | 0.68              |
| 25:L:42:TRP:HZ2  | 25:L:102:MET:SD   | 2.17                     | 0.68              |
| 40:a:1056:G:O2'  | 40:a:1103:A:N6    | 2.27                     | 0.68              |
| 1:0:52:PRO:HB3   | 65:z:89:GLU:OE2   | 1.94                     | 0.68              |
| 17:D:673:A:H5''  | 25:L:86:ARG:NH1   | 2.09                     | 0.68              |
| 19:F:12:PHE:CE1  | 30:Q:107:ILE:HG22 | 2.29                     | 0.68              |
| 21:H:23:ILE:N    | 21:H:69:ASP:OD2   | 2.27                     | 0.68              |
| 33:T:27:VAL:O    | 33:T:31:LEU:HD23  | 1.93                     | 0.68              |
| 40:a:2314:A:H1'  | 53:n:155:THR:HG21 | 1.74                     | 0.68              |
| 51:l:101:TYR:CE2 | 51:l:105:LEU:HD11 | 2.28                     | 0.68              |
| 7:6:25:DT:H2'    | 11:AA:496:LYS:HG3 | 1.73                     | 0.68              |
| 10:A:58:A:O2'    | 10:A:59:A:H3'     | 1.93                     | 0.68              |
| 22:I:134:MET:HE1 | 22:I:167:TRP:HA   | 1.76                     | 0.68              |
| 25:L:18:VAL:HA   | 25:L:21:MET:HE2   | 1.75                     | 0.68              |
| 26:M:109:ARG:HD2 | 26:M:116:MET:HE1  | 1.76                     | 0.68              |
| 59:t:9:ASN:OD1   | 59:t:10:VAL:N     | 2.27                     | 0.68              |
| 61:v:1:MET:HE1   | 61:v:44:ARG:N     | 2.09                     | 0.68              |
| 5:4:77:VAL:HG23  | 5:4:89:ILE:HG12   | 1.76                     | 0.68              |
| 9:9:92:ALA:HB1   | 9:9:129:LEU:HD22  | 1.74                     | 0.68              |
| 11:AA:65:ASN:HB3 | 11:AA:105:TYR:HB2 | 1.73                     | 0.68              |
| 19:F:8:GLU:OE2   | 19:F:9:ASN:ND2    | 2.26                     | 0.68              |
| 38:Y:116:MET:HG2 | 38:Y:124:MET:CG   | 2.24                     | 0.68              |
| 9:9:44:ALA:HA    | 9:9:47:GLU:OE1    | 1.94                     | 0.67              |
| 17:D:588:G:H4'   | 27:N:3:MET:HE1    | 1.76                     | 0.67              |
| 36:W:36:ARG:NH2  | 36:W:75:ALA:O     | 2.26                     | 0.67              |
| 40:a:2420:C:H5'' | 50:k:8:LYS:CE     | 2.25                     | 0.67              |
| 7:6:18:DT:N3     | 8:7:34:A:N6       | 2.36                     | 0.67              |
| 9:9:43:LYS:NZ    | 9:9:101:LYS:HE2   | 2.09                     | 0.67              |
| 9:9:47:GLU:HG3   | 9:9:94:ARG:CZ     | 2.24                     | 0.67              |
| 12:AB:34:THR:HA  | 12:AB:47:SER:HA   | 1.76                     | 0.67              |
| 18:E:79:LEU:HA   | 18:E:82:GLN:OE1   | 1.94                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:M:20:SER:CB    | 26:M:23:LEU:HD13   | 2.24                     | 0.67              |
| 39:Z:20:VAL:O     | 39:Z:20:VAL:HG12   | 1.94                     | 0.67              |
| 5:4:75:GLN:HG3    | 5:4:92:VAL:CG2     | 2.24                     | 0.67              |
| 31:R:27:CYS:HB2   | 31:R:30:LYS:HE2    | 1.75                     | 0.67              |
| 38:Y:32:VAL:HG22  | 38:Y:60:VAL:HG21   | 1.76                     | 0.67              |
| 51:l:118:LEU:HD11 | 51:l:188:MET:SD    | 2.35                     | 0.67              |
| 65:z:68:ALA:HB1   | 65:z:106:PHE:CE2   | 2.29                     | 0.67              |
| 65:z:79:PHE:HE1   | 65:z:110:VAL:HA    | 1.60                     | 0.67              |
| 5:4:89:ILE:HG21   | 5:4:91:PHE:CE1     | 2.29                     | 0.67              |
| 9:9:139:LEU:HD21  | 39:Z:11:VAL:HG22   | 1.76                     | 0.67              |
| 13:AD:48:LEU:HB2  | 13:AD:183:ILE:HD11 | 1.76                     | 0.67              |
| 16:C:13:PHE:HB3   | 16:C:51:TYR:CE1    | 2.30                     | 0.67              |
| 17:D:274:A:H4'    | 35:V:16:LYS:HE3    | 1.76                     | 0.67              |
| 17:D:876:C:H1'    | 27:N:12:THR:HG21   | 1.76                     | 0.67              |
| 21:H:304:VAL:O    | 21:H:304:VAL:HG12  | 1.94                     | 0.67              |
| 22:I:134:MET:HE3  | 22:I:151:VAL:HG23  | 1.75                     | 0.67              |
| 25:L:38:ARG:NH1   | 25:L:99:ALA:HB2    | 2.09                     | 0.67              |
| 32:S:19:LYS:HG3   | 32:S:20:TYR:CD1    | 2.29                     | 0.67              |
| 38:Y:85:ILE:H     | 38:Y:85:ILE:HD12   | 1.59                     | 0.67              |
| 40:a:111:A:O3'    | 44:e:58:ASN:ND2    | 2.28                     | 0.67              |
| 47:h:76:ALA:HB1   | 47:h:94:VAL:HG12   | 1.76                     | 0.67              |
| 51:l:6:LYS:HE3    | 51:l:119:ILE:HG23  | 1.75                     | 0.67              |
| 9:9:73:LYS:HG2    | 9:9:117:LEU:HD12   | 1.76                     | 0.67              |
| 10:B:75:C:OP2     | 40:a:2602:A:C2'    | 2.43                     | 0.67              |
| 17:D:564:C:OP1    | 31:R:12:ARG:NH1    | 2.27                     | 0.67              |
| 37:X:81:MET:CE    | 40:a:888:C:C5      | 2.78                     | 0.67              |
| 40:a:2420:C:H5''  | 50:k:8:LYS:NZ      | 2.09                     | 0.67              |
| 62:w:24:MET:HE2   | 62:w:34:ILE:CD1    | 2.24                     | 0.67              |
| 17:D:1308:U:P     | 37:X:100:GLN:HE22  | 2.16                     | 0.67              |
| 20:G:100:MET:HE1  | 20:G:101:LEU:HD21  | 1.75                     | 0.67              |
| 23:J:121:LYS:HG2  | 23:J:131:ASN:HD21  | 1.59                     | 0.67              |
| 40:a:666:A:H1'    | 54:o:4:ILE:HD12    | 1.76                     | 0.67              |
| 57:r:37:VAL:HG12  | 57:r:43:ASN:ND2    | 2.09                     | 0.67              |
| 5:4:56:PHE:O      | 5:4:61:LEU:HD11    | 1.95                     | 0.67              |
| 12:AB:89:PRO:CG   | 14:AE:290:ILE:HG21 | 2.24                     | 0.67              |
| 17:D:945:G:C2     | 17:D:946:A:C8      | 2.83                     | 0.67              |
| 21:H:308:GLU:O    | 21:H:310:ASP:N     | 2.26                     | 0.67              |
| 33:T:80:GLN:O     | 33:T:83:GLU:HG3    | 1.95                     | 0.67              |
| 40:a:1665:A:O5'   | 59:t:66:LYS:NZ     | 2.28                     | 0.67              |
| 61:v:1:MET:HE1    | 61:v:44:ARG:HA     | 1.76                     | 0.67              |
| 8:7:8:U:H5'       | 17:D:1397:C:N3     | 2.10                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:9:24:SER:CB     | 9:9:116:GLU:HG3   | 2.24                     | 0.67              |
| 10:B:24:U:O2'     | 40:a:1922:G:O3'   | 2.12                     | 0.67              |
| 40:a:1802:A:H2'   | 40:a:1803:A:C8    | 2.30                     | 0.67              |
| 40:a:2682:A:C8    | 49:j:11:MET:HE1   | 2.30                     | 0.67              |
| 47:h:129:THR:HG22 | 47:h:189:ARG:HD2  | 1.77                     | 0.67              |
| 17:D:1151:A:HO2'  | 17:D:1152:A:P     | 2.18                     | 0.67              |
| 18:E:25:ARG:HD2   | 18:E:66:LEU:HD11  | 1.75                     | 0.67              |
| 37:X:90:ARG:HD2   | 37:X:97:VAL:HA    | 1.77                     | 0.67              |
| 38:Y:23:VAL:HG23  | 38:Y:24:GLY:H     | 1.58                     | 0.67              |
| 40:a:2682:A:O4'   | 49:j:11:MET:HE1   | 1.95                     | 0.67              |
| 49:j:3:GLY:O      | 49:j:4:LEU:HD12   | 1.95                     | 0.67              |
| 12:AB:27:ASN:CG   | 12:AB:58:GLU:HB2  | 2.20                     | 0.66              |
| 16:C:70:TYR:CE2   | 17:D:674:G:H4'    | 2.30                     | 0.66              |
| 40:a:927:A:H2'    | 40:a:928:A:C8     | 2.30                     | 0.66              |
| 58:s:13:ARG:HH22  | 58:s:50:THR:HA    | 1.60                     | 0.66              |
| 17:D:1228:C:OP2   | 37:X:110:LYS:NZ   | 2.28                     | 0.66              |
| 19:F:31:GLU:OE1   | 19:F:34:ARG:NH2   | 2.28                     | 0.66              |
| 24:K:156:LYS:HE3  | 27:N:71:VAL:HG13  | 1.76                     | 0.66              |
| 32:S:42:TRP:HH2   | 46:g:66:ILE:HA    | 1.61                     | 0.66              |
| 40:a:1454:C:O4'   | 62:w:63:ARG:NE    | 2.28                     | 0.66              |
| 45:f:41:THR:O     | 45:f:44:ILE:HG22  | 1.94                     | 0.66              |
| 17:D:43:C:OP1     | 34:U:12:LYS:NZ    | 2.29                     | 0.66              |
| 38:Y:37:PHE:CZ    | 38:Y:56:VAL:HG11  | 2.30                     | 0.66              |
| 53:n:93:GLY:O     | 53:n:96:MET:N     | 2.29                     | 0.66              |
| 55:p:85:LYS:CE    | 55:p:164:TYR:HD1  | 2.07                     | 0.66              |
| 62:w:49:GLU:OE1   | 62:w:49:GLU:N     | 2.26                     | 0.66              |
| 10:A:32:C:H4'     | 26:M:86:GLN:NE2   | 2.10                     | 0.66              |
| 27:N:67:GLN:OE1   | 27:N:67:GLN:N     | 2.28                     | 0.66              |
| 36:W:62:VAL:HG13  | 36:W:66:MET:HE3   | 1.77                     | 0.66              |
| 38:Y:102:ARG:NE   | 38:Y:102:ARG:HA   | 2.11                     | 0.66              |
| 40:a:1816:C:N4    | 47:h:35:GLU:OE2   | 2.20                     | 0.66              |
| 59:t:112:PHE:HD2  | 59:t:115:ILE:HD12 | 1.59                     | 0.66              |
| 10:A:71:C:H3'     | 10:A:72:A:C8      | 2.30                     | 0.66              |
| 47:h:52:ARG:HE    | 47:h:53:HIS:HE1   | 1.43                     | 0.66              |
| 59:t:38:ILE:HD11  | 59:t:112:PHE:HZ   | 1.60                     | 0.66              |
| 9:9:14:GLU:O      | 9:9:18:VAL:HG23   | 1.96                     | 0.66              |
| 12:AB:81:PHE:HE1  | 14:AE:293:ARG:HB3 | 0.85                     | 0.66              |
| 16:C:51:TYR:CD1   | 16:C:54:GLN:NE2   | 2.64                     | 0.66              |
| 19:F:58:LYS:O     | 19:F:62:ARG:HG2   | 1.96                     | 0.66              |
| 20:G:101:LEU:HD22 | 20:G:157:LEU:CD1  | 2.26                     | 0.66              |
| 42:c:71:LEU:HB3   | 42:c:76:GLU:CD    | 2.20                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:l:40:ARG:HD2   | 51:l:92:HIS:ND1   | 2.11                     | 0.66              |
| 56:q:1:MET:HE1    | 56:q:35:GLN:CA    | 2.25                     | 0.66              |
| 9:9:23:LEU:HD13   | 9:9:92:ALA:HB2    | 1.77                     | 0.66              |
| 10:B:75:C:P       | 40:a:2602:A:HO2'  | 2.13                     | 0.66              |
| 20:G:53:ALA:HA    | 20:G:56:GLU:OE1   | 1.96                     | 0.66              |
| 5:4:84:PRO:O      | 5:4:85:LYS:HE2    | 1.96                     | 0.66              |
| 9:9:139:LEU:CD2   | 39:Z:11:VAL:HG22  | 2.26                     | 0.66              |
| 26:M:23:LEU:HD21  | 26:M:59:LEU:HD21  | 1.76                     | 0.66              |
| 26:M:26:PHE:HD1   | 26:M:101:MET:SD   | 2.19                     | 0.66              |
| 58:s:15:TRP:NE1   | 58:s:53:TYR:CD2   | 2.63                     | 0.66              |
| 6:5:9:DG:O5'      | 11:AA:473:ARG:HB3 | 1.95                     | 0.66              |
| 18:E:54:MET:HE1   | 18:E:75:HIS:CE1   | 2.31                     | 0.66              |
| 22:I:151:VAL:HG12 | 22:I:200:VAL:HG23 | 1.77                     | 0.66              |
| 38:Y:79:LEU:HD21  | 38:Y:105:LEU:CD2  | 2.24                     | 0.66              |
| 40:a:752:A:OP1    | 52:m:1:MET:HE1    | 1.95                     | 0.66              |
| 45:f:40:ASP:C     | 45:f:45:ARG:HH22  | 2.03                     | 0.66              |
| 9:9:25:ALA:HB3    | 9:9:99:PHE:HD2    | 1.61                     | 0.66              |
| 12:AB:129:ILE:O   | 12:AB:142:LEU:CB  | 2.44                     | 0.66              |
| 18:E:21:ASN:C     | 18:E:25:ARG:NE    | 2.54                     | 0.66              |
| 20:G:90:PHE:CE2   | 20:G:154:MET:HE3  | 2.31                     | 0.66              |
| 38:Y:102:ARG:HG3  | 38:Y:140:GLU:O    | 1.96                     | 0.66              |
| 40:a:2334:U:H4'   | 40:a:2335:A:OP2   | 1.95                     | 0.66              |
| 6:5:10:DT:H73     | 11:AA:62:TYR:CB   | 2.25                     | 0.65              |
| 9:9:28:ALA:H      | 9:9:110:ALA:HA    | 1.61                     | 0.65              |
| 17:D:280:C:H1'    | 35:V:40:ARG:NH2   | 2.11                     | 0.65              |
| 20:G:134:ALA:O    | 20:G:137:ARG:HG2  | 1.96                     | 0.65              |
| 21:H:163:ARG:N    | 21:H:298:GLU:OE2  | 2.28                     | 0.65              |
| 26:M:46:ALA:CB    | 26:M:120:LEU:HD22 | 2.25                     | 0.65              |
| 37:X:28:THR:HA    | 37:X:31:LYS:HE3   | 1.78                     | 0.65              |
| 40:a:614:A:O2'    | 40:a:615:U:OP2    | 2.12                     | 0.65              |
| 59:t:1:MET:HE1    | 59:t:32:TYR:CG    | 2.31                     | 0.65              |
| 61:v:111:GLU:HG2  | 61:v:112:LEU:HD12 | 1.78                     | 0.65              |
| 12:AB:155:LYS:HG3 | 12:AB:156:ASN:H   | 1.62                     | 0.65              |
| 14:AE:58:CYS:SG   | 14:AE:59:ALA:N    | 2.69                     | 0.65              |
| 17:D:246:A:C2     | 17:D:282:A:C5     | 2.84                     | 0.65              |
| 20:G:90:PHE:CD2   | 20:G:154:MET:HE3  | 2.31                     | 0.65              |
| 23:J:196:ASN:OD1  | 23:J:198:HIS:CE1  | 2.49                     | 0.65              |
| 38:Y:45:THR:HG21  | 38:Y:50:LYS:HD3   | 1.76                     | 0.65              |
| 40:a:2355:G:C2'   | 40:a:2356:U:H5'   | 2.26                     | 0.65              |
| 50:k:21:TYR:OH    | 50:k:39:PHE:O     | 2.10                     | 0.65              |
| 61:v:45:GLN:NE2   | 61:v:125:PRO:HD3  | 2.10                     | 0.65              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 6:5:10:DT:C7      | 11:AA:62:TYR:CB     | 2.74                     | 0.65              |
| 40:a:1596:A:H2'   | 40:a:1597:A:C8      | 2.32                     | 0.65              |
| 59:t:99:ILE:HD13  | 59:t:118:LEU:HB2    | 1.77                     | 0.65              |
| 6:5:11:DA:H5'     | 12:AB:67:THR:CB     | 2.27                     | 0.65              |
| 8:7:29:U:C5'      | 11:AA:1259:LEU:HD21 | 2.27                     | 0.65              |
| 9:9:24:SER:OG     | 9:9:86:MET:HE2      | 1.96                     | 0.65              |
| 12:AB:115:LYS:HD3 | 12:AB:129:ILE:HD12  | 1.77                     | 0.65              |
| 20:G:23:TRP:CD1   | 20:G:39:HIS:HE1     | 2.14                     | 0.65              |
| 38:Y:81:LYS:NZ    | 38:Y:86:LYS:HE2     | 2.12                     | 0.65              |
| 40:a:1800:C:OP2   | 47:h:182:ARG:NH1    | 2.27                     | 0.65              |
| 40:a:2572:A:N7    | 49:j:150:GLN:NE2    | 2.45                     | 0.65              |
| 54:o:30:ARG:HH12  | 60:u:62:PRO:CB      | 2.10                     | 0.65              |
| 61:v:45:GLN:NE2   | 61:v:125:PRO:CD     | 2.59                     | 0.65              |
| 1:0:55:ASP:OD1    | 1:0:56:GLY:N        | 2.27                     | 0.65              |
| 12:AB:9:CYS:HB3   | 12:AB:74:GLY:HA2    | 1.79                     | 0.65              |
| 12:AB:129:ILE:H   | 12:AB:142:LEU:HB3   | 1.60                     | 0.65              |
| 14:AE:84:ILE:HG22 | 14:AE:91:GLU:HG3    | 1.78                     | 0.65              |
| 16:C:73:ARG:HH12  | 30:Q:113:VAL:CB     | 2.09                     | 0.65              |
| 17:D:375:U:P      | 34:U:70:ARG:NE      | 2.69                     | 0.65              |
| 38:Y:5:GLN:HG2    | 38:Y:61:TYR:CD1     | 2.32                     | 0.65              |
| 51:l:45:ALA:HB1   | 51:l:88:ARG:NH2     | 2.12                     | 0.65              |
| 55:p:52:PHE:CD1   | 55:p:69:ARG:HD3     | 2.32                     | 0.65              |
| 59:t:1:MET:HE1    | 59:t:32:TYR:CD1     | 2.31                     | 0.65              |
| 3:2:9:LYS:O       | 3:2:12:ARG:NH1      | 2.30                     | 0.65              |
| 6:5:16:DG:H1      | 11:AA:451:ARG:NH2   | 1.94                     | 0.65              |
| 8:7:38:G:OP1      | 11:AA:1073:LYS:NZ   | 2.24                     | 0.65              |
| 17:D:1158:C:O2'   | 20:G:132:LYS:CE     | 2.45                     | 0.65              |
| 18:E:28:MET:SD    | 18:E:61:GLN:HG3     | 2.36                     | 0.65              |
| 28:O:86:ALA:O     | 28:O:89:GLU:HG2     | 1.95                     | 0.65              |
| 38:Y:24:GLY:O     | 38:Y:27:LEU:HG      | 1.96                     | 0.65              |
| 40:a:1839:G:H1'   | 40:a:1927:A:C8      | 2.32                     | 0.65              |
| 40:a:2682:A:H2'   | 40:a:2683:C:O4'     | 1.96                     | 0.65              |
| 43:d:55:U:H1'     | 53:n:26:MET:CE      | 2.26                     | 0.65              |
| 51:l:62:GLN:O     | 51:l:69:ARG:NE      | 2.30                     | 0.65              |
| 58:s:43:GLU:OE1   | 58:s:43:GLU:N       | 2.29                     | 0.65              |
| 59:t:42:THR:HG23  | 59:t:44:LYS:NZ      | 2.12                     | 0.65              |
| 10:A:76:A:N6      | 40:a:2422:C:O5'     | 2.29                     | 0.65              |
| 10:B:71:C:H3'     | 10:B:72:A:C8        | 2.30                     | 0.65              |
| 17:D:1308:U:P     | 37:X:100:GLN:NE2    | 2.70                     | 0.65              |
| 28:O:83:ILE:O     | 28:O:87:LEU:HD23    | 1.96                     | 0.65              |
| 46:g:58:ASP:C     | 46:g:62:LYS:NZ      | 2.55                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 61:v:31:PHE:N     | 61:v:104:GLU:OE2  | 2.30                     | 0.65              |
| 65:z:41:LYS:HG3   | 65:z:45:TYR:CE2   | 2.32                     | 0.65              |
| 65:z:85:LYS:HD2   | 65:z:116:ALA:HB1  | 1.78                     | 0.65              |
| 3:2:3:ARG:NH1     | 3:2:5:GLU:OE2     | 2.30                     | 0.65              |
| 9:9:47:GLU:HG2    | 9:9:95:LEU:HD21   | 1.78                     | 0.65              |
| 20:G:26:LYS:NZ    | 20:G:193:PRO:HG2  | 2.12                     | 0.65              |
| 21:H:277:GLY:HA2  | 21:H:331:MET:CE   | 2.27                     | 0.65              |
| 27:N:10:MET:HG3   | 27:N:27:MET:HE1   | 1.78                     | 0.65              |
| 35:V:60:GLU:OE1   | 35:V:76:VAL:CG2   | 2.45                     | 0.65              |
| 40:a:1824:G:OP1   | 47:h:52:ARG:CZ    | 2.44                     | 0.65              |
| 40:a:2175:C:H2'   | 40:a:2176:A:C8    | 2.31                     | 0.65              |
| 40:a:2356:U:O3'   | 41:b:20:ARG:CZ    | 2.45                     | 0.65              |
| 42:c:66:THR:HG22  | 42:c:70:GLU:OE2   | 1.97                     | 0.65              |
| 58:s:53:TYR:CE1   | 58:s:121:LYS:HD2  | 2.32                     | 0.65              |
| 2:1:71:VAL:HB     | 2:1:74:ILE:HD11   | 1.79                     | 0.65              |
| 5:4:50:MET:HB3    | 5:4:56:PHE:CE1    | 2.31                     | 0.65              |
| 12:AB:129:ILE:O   | 12:AB:142:LEU:HB2 | 1.97                     | 0.65              |
| 12:AB:136:GLU:O   | 12:AB:156:ASN:HA  | 1.97                     | 0.65              |
| 31:R:30:LYS:HB3   | 31:R:57:LEU:HD11  | 1.78                     | 0.65              |
| 46:g:58:ASP:C     | 46:g:62:LYS:HZ3   | 2.05                     | 0.65              |
| 9:9:25:ALA:HB2    | 9:9:96:PHE:CE1    | 2.31                     | 0.65              |
| 16:C:34:THR:N     | 16:C:38:LYS:O     | 2.30                     | 0.65              |
| 17:D:1151:A:O2'   | 17:D:1152:A:O5'   | 2.13                     | 0.65              |
| 38:Y:20:SER:HB2   | 38:Y:21:PRO:HD3   | 1.79                     | 0.65              |
| 40:a:1278:C:C4'   | 62:w:24:MET:HE1   | 2.27                     | 0.65              |
| 51:l:147:LEU:HB2  | 51:l:183:PHE:HD2  | 1.62                     | 0.65              |
| 55:p:107:LEU:O    | 55:p:152:ARG:CZ   | 2.45                     | 0.65              |
| 61:v:105:MET:CE   | 61:v:108:VAL:HG21 | 2.27                     | 0.65              |
| 9:9:43:LYS:HD3    | 9:9:98:GLU:HG3    | 1.78                     | 0.64              |
| 19:F:58:LYS:O     | 19:F:62:ARG:CG    | 2.45                     | 0.64              |
| 20:G:114:LEU:HD13 | 20:G:144:LEU:CB   | 2.28                     | 0.64              |
| 21:H:303:LEU:O    | 21:H:303:LEU:HG   | 1.96                     | 0.64              |
| 21:H:308:GLU:HG2  | 21:H:309:MET:H    | 1.61                     | 0.64              |
| 23:J:138:SER:O    | 23:J:141:ASP:CG   | 2.40                     | 0.64              |
| 23:J:150:LYS:HE2  | 23:J:178:MET:HE2  | 1.79                     | 0.64              |
| 32:S:53:ARG:HB3   | 32:S:59:ARG:NH1   | 2.11                     | 0.64              |
| 38:Y:126:ARG:NH2  | 40:a:1083:U:P     | 2.70                     | 0.64              |
| 39:Z:22:LEU:O     | 39:Z:26:MET:HE1   | 1.97                     | 0.64              |
| 57:r:137:GLU:HG2  | 57:r:138:VAL:N    | 2.11                     | 0.64              |
| 60:u:122:VAL:CG1  | 60:u:125:LEU:HD11 | 2.27                     | 0.64              |
| 12:AB:139:SER:C   | 12:AB:152:HIS:O   | 2.40                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:K:61:GLN:HA    | 24:K:64:MET:CE    | 2.27                     | 0.64              |
| 24:K:148:ASN:OD1  | 27:N:96:MET:CE    | 2.45                     | 0.64              |
| 28:O:5:GLN:NE2    | 28:O:20:PHE:HB3   | 2.10                     | 0.64              |
| 51:l:149:ILE:HD11 | 51:l:188:MET:HG2  | 1.78                     | 0.64              |
| 4:3:26:LYS:HB2    | 4:3:35:ILE:HG23   | 1.78                     | 0.64              |
| 10:B:22:G:H2'     | 10:B:23:C:C6      | 2.32                     | 0.64              |
| 26:M:23:LEU:HD12  | 26:M:23:LEU:N     | 2.13                     | 0.64              |
| 33:T:64:ARG:NH1   | 33:T:89:ARG:HH22  | 1.94                     | 0.64              |
| 38:Y:5:GLN:HE22   | 38:Y:60:VAL:N     | 1.96                     | 0.64              |
| 38:Y:14:ALA:HB3   | 38:Y:51:GLY:N     | 2.12                     | 0.64              |
| 38:Y:14:ALA:C     | 38:Y:50:LYS:HE3   | 2.22                     | 0.64              |
| 40:a:998:C:OP2    | 65:z:92:ARG:NH2   | 2.29                     | 0.64              |
| 45:f:10:THR:HB    | 45:f:56:LYS:HZ2   | 1.63                     | 0.64              |
| 47:h:53:HIS:NE2   | 47:h:219:THR:HA   | 2.11                     | 0.64              |
| 51:l:194:LYS:O    | 51:l:198:GLU:OE1  | 2.15                     | 0.64              |
| 5:4:57:TYR:OH     | 5:4:79:ARG:NH2    | 2.24                     | 0.64              |
| 10:A:32:C:H4'     | 26:M:86:GLN:HE21  | 1.62                     | 0.64              |
| 14:AE:79:LYS:C    | 14:AE:81:ARG:CZ   | 2.71                     | 0.64              |
| 23:J:62:ARG:HG2   | 23:J:72:PHE:CZ    | 2.33                     | 0.64              |
| 26:M:23:LEU:HD21  | 26:M:59:LEU:CD2   | 2.27                     | 0.64              |
| 32:S:87:ALA:CA    | 32:S:90:ARG:NH1   | 2.60                     | 0.64              |
| 33:T:53:ARG:O     | 33:T:57:LEU:HD23  | 1.97                     | 0.64              |
| 34:U:5:ARG:HG2    | 34:U:68:SER:HB2   | 1.80                     | 0.64              |
| 37:X:16:VAL:HG23  | 37:X:17:ILE:HD12  | 1.80                     | 0.64              |
| 38:Y:79:LEU:CD2   | 38:Y:105:LEU:HD21 | 2.27                     | 0.64              |
| 38:Y:102:ARG:HD2  | 38:Y:141:ASP:CB   | 2.27                     | 0.64              |
| 40:a:2308:G:C5    | 53:n:77:PHE:CZ    | 2.85                     | 0.64              |
| 8:7:9:U:N3        | 17:D:1196:A:N7    | 2.45                     | 0.64              |
| 38:Y:102:ARG:NE   | 38:Y:139:VAL:HG21 | 2.13                     | 0.64              |
| 40:a:2723:C:H5''  | 62:w:1:MET:HE3    | 1.78                     | 0.64              |
| 8:7:11:U:C4'      | 24:K:20:ARG:HH22  | 1.93                     | 0.64              |
| 10:A:22:G:H2'     | 10:A:23:C:C6      | 2.32                     | 0.64              |
| 19:F:10:GLU:OE2   | 19:F:18:ARG:NE    | 2.30                     | 0.64              |
| 20:G:49:MET:HE1   | 20:G:201:PRO:CD   | 2.23                     | 0.64              |
| 21:H:70:VAL:HG12  | 21:H:83:LEU:O     | 1.98                     | 0.64              |
| 21:H:119:GLY:HA2  | 21:H:133:GLY:HA2  | 1.80                     | 0.64              |
| 32:S:87:ALA:HA    | 32:S:90:ARG:CZ    | 2.28                     | 0.64              |
| 53:n:117:LEU:HD13 | 53:n:176:PRO:CG   | 2.26                     | 0.64              |
| 9:9:47:GLU:HB3    | 9:9:51:TYR:OH     | 1.97                     | 0.64              |
| 9:9:56:ARG:H      | 9:9:56:ARG:HD3    | 1.63                     | 0.64              |
| 17:D:1323:G:H2'   | 17:D:1324:A:C8    | 2.33                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:E:16:LYS:O     | 18:E:19:LYS:HG2    | 1.97                     | 0.64              |
| 25:L:2:ARG:CZ     | 25:L:68:GLN:NE2    | 2.60                     | 0.64              |
| 40:a:1067:A:O2'   | 40:a:1068:G:O4'    | 2.16                     | 0.64              |
| 53:n:135:GLN:HG3  | 53:n:150:ARG:NH2   | 2.12                     | 0.64              |
| 55:p:149:ARG:CZ   | 55:p:162:VAL:O     | 2.45                     | 0.64              |
| 8:7:25:G:O2'      | 14:AE:394:ILE:HG21 | 1.97                     | 0.64              |
| 9:9:117:LEU:O     | 9:9:117:LEU:HD23   | 1.98                     | 0.64              |
| 10:A:54:U:H3      | 10:A:58:A:N6       | 1.96                     | 0.64              |
| 17:D:675:A:H1'    | 30:Q:118:HIS:CD2   | 2.33                     | 0.64              |
| 22:I:132:ARG:O    | 22:I:135:LYS:HG2   | 1.97                     | 0.64              |
| 31:R:80:ILE:HD12  | 31:R:104:CYS:HB2   | 1.79                     | 0.64              |
| 33:T:3:LEU:HD22   | 33:T:8:THR:CG2     | 2.28                     | 0.64              |
| 35:V:31:HIS:CD2   | 35:V:34:TYR:H      | 2.15                     | 0.64              |
| 38:Y:21:PRO:HB2   | 38:Y:22:PRO:HD3    | 1.80                     | 0.64              |
| 40:a:617:G:H4'    | 51:l:199:MET:HE1   | 1.78                     | 0.64              |
| 10:A:19:G:C2      | 40:a:2112:G:O4'    | 2.50                     | 0.64              |
| 11:AA:387:ASN:HB3 | 11:AA:394:ARG:HH11 | 1.63                     | 0.64              |
| 10:B:76:A:H1'     | 40:a:2494:G:OP1    | 1.98                     | 0.64              |
| 24:K:111:MET:HE1  | 24:K:125:ALA:HB1   | 1.80                     | 0.64              |
| 32:S:10:GLU:O     | 32:S:14:VAL:HG23   | 1.97                     | 0.64              |
| 63:x:114:GLY:O    | 63:x:116:GLN:NE2   | 2.31                     | 0.64              |
| 12:AB:31:PRO:HB2  | 12:AB:50:LEU:HB3   | 1.80                     | 0.64              |
| 14:AE:288:PRO:HD2 | 14:AE:291:ILE:HG22 | 1.74                     | 0.64              |
| 16:C:73:ARG:HH12  | 30:Q:113:VAL:HA    | 1.62                     | 0.64              |
| 17:D:714:G:H2'    | 17:D:715:A:C8      | 2.32                     | 0.64              |
| 20:G:27:MET:HG2   | 20:G:189:THR:HA    | 1.78                     | 0.64              |
| 23:J:74:ASN:HA    | 23:J:77:LYS:HZ3    | 1.62                     | 0.64              |
| 25:L:25:TYR:O     | 25:L:29:ILE:HD12   | 1.97                     | 0.64              |
| 33:T:88:ARG:NH2   | 40:a:714:U:OP2     | 2.31                     | 0.64              |
| 38:Y:31:GLY:C     | 38:Y:60:VAL:HG11   | 2.23                     | 0.64              |
| 38:Y:86:LYS:HD3   | 38:Y:86:LYS:C      | 2.23                     | 0.64              |
| 9:9:100:ALA:HB2   | 9:9:125:ARG:NE     | 2.13                     | 0.63              |
| 17:D:738:C:H5''   | 25:L:68:GLN:NE2    | 2.12                     | 0.63              |
| 38:Y:99:LYS:HD2   | 38:Y:140:GLU:CD    | 2.22                     | 0.63              |
| 40:a:196:A:C2     | 60:u:50:PHE:HZ     | 2.16                     | 0.63              |
| 40:a:2311:A:N3    | 53:n:85:ILE:HD11   | 2.13                     | 0.63              |
| 40:a:2335:A:P     | 63:x:13:ARG:CZ     | 2.87                     | 0.63              |
| 4:3:34:VAL:HG13   | 4:3:67:VAL:HG22    | 1.78                     | 0.63              |
| 10:B:54:U:H3      | 10:B:58:A:N6       | 1.96                     | 0.63              |
| 22:I:156:ARG:HH11 | 22:I:193:TYR:HB3   | 1.63                     | 0.63              |
| 32:S:77:PHE:HE1   | 32:S:93:ILE:HG21   | 1.63                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:a:537:G:OP1     | 58:s:2:LYS:HE2     | 1.98                     | 0.63              |
| 40:a:2393:U:P      | 54:o:30:ARG:NE     | 2.70                     | 0.63              |
| 47:h:251:GLN:HE22  | 47:h:253:LYS:C     | 2.07                     | 0.63              |
| 51:l:112:LEU:HG    | 51:l:118:LEU:HB2   | 1.79                     | 0.63              |
| 16:C:13:PHE:CE2    | 16:C:21:ILE:HD11   | 2.34                     | 0.63              |
| 64:y:31:TRP:CZ3    | 64:y:38:LYS:HD3    | 2.33                     | 0.63              |
| 1:0:84:ARG:NH1     | 40:a:813:U:OP1     | 2.31                     | 0.63              |
| 2:1:25:ARG:NH2     | 40:a:520:G:C5'     | 2.60                     | 0.63              |
| 11:AA:1282:GLY:HA3 | 15:AF:17:PHE:HE1   | 1.63                     | 0.63              |
| 14:AE:79:LYS:C     | 14:AE:81:ARG:NH2   | 2.56                     | 0.63              |
| 38:Y:48:ILE:HG13   | 38:Y:49:GLU:N      | 2.10                     | 0.63              |
| 38:Y:55:PRO:HB2    | 38:Y:71:LYS:HE2    | 1.80                     | 0.63              |
| 40:a:2682:A:O5'    | 49:j:11:MET:HE1    | 1.98                     | 0.63              |
| 48:i:17:ARG:HA     | 48:i:20:ASP:OD1    | 1.99                     | 0.63              |
| 1:0:51:VAL:HG23    | 65:z:86:ALA:O      | 1.98                     | 0.63              |
| 8:7:9:U:N3         | 17:D:1196:A:C8     | 2.66                     | 0.63              |
| 9:9:24:SER:OG      | 9:9:116:GLU:HG3    | 1.98                     | 0.63              |
| 12:AB:80:ARG:HB3   | 12:AB:82:GLY:O     | 1.99                     | 0.63              |
| 20:G:19:GLN:HG3    | 21:H:76:GLU:HB3    | 1.79                     | 0.63              |
| 40:a:2013:A:N1     | 40:a:2613:U:O4     | 2.32                     | 0.63              |
| 3:2:36:LYS:HE3     | 3:2:79:ASP:OD2     | 1.98                     | 0.63              |
| 12:AB:117:ILE:O    | 12:AB:118:ILE:HG13 | 1.98                     | 0.63              |
| 31:R:25:GLU:CD     | 31:R:59:ASN:HD22   | 2.05                     | 0.63              |
| 36:W:66:MET:SD     | 36:W:66:MET:O      | 2.57                     | 0.63              |
| 38:Y:37:PHE:CE1    | 38:Y:56:VAL:HG11   | 2.33                     | 0.63              |
| 60:u:84:LYS:HZ2    | 60:u:98:ALA:C      | 2.02                     | 0.63              |
| 1:0:82:HIS:CG      | 1:0:82:HIS:O       | 2.52                     | 0.63              |
| 6:5:11:DA:P        | 12:AB:67:THR:C     | 2.79                     | 0.63              |
| 9:9:77:VAL:HG12    | 9:9:77:VAL:O       | 1.99                     | 0.63              |
| 12:AB:129:ILE:HB   | 12:AB:142:LEU:CD2  | 2.28                     | 0.63              |
| 12:AB:147:ASN:CA   | 29:P:100:ILE:HG23  | 2.26                     | 0.63              |
| 40:a:2419:U:H4'    | 50:k:22:THR:HG21   | 1.78                     | 0.63              |
| 5:4:50:MET:O       | 5:4:52:ALA:N       | 2.31                     | 0.63              |
| 9:9:7:ASP:O        | 9:9:11:ILE:HD12    | 1.98                     | 0.63              |
| 17:D:1226:C:H2'    | 37:X:102:THR:OG1   | 1.98                     | 0.63              |
| 38:Y:100:ILE:CD1   | 38:Y:139:VAL:HB    | 2.29                     | 0.63              |
| 51:l:69:ARG:NH1    | 51:l:69:ARG:HA     | 2.13                     | 0.63              |
| 53:n:33:LYS:HA     | 53:n:96:MET:SD     | 2.39                     | 0.63              |
| 63:x:90:VAL:HG21   | 63:x:115:LEU:HD21  | 1.81                     | 0.63              |
| 9:9:73:LYS:NZ      | 9:9:115:GLY:O      | 2.31                     | 0.63              |
| 20:G:118:GLU:O     | 20:G:121:SER:OG    | 2.15                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:K:61:GLN:HA     | 24:K:64:MET:HE3   | 1.81                     | 0.63              |
| 24:K:137:VAL:O     | 24:K:140:THR:OG1  | 2.15                     | 0.63              |
| 32:S:13:ARG:HB3    | 32:S:60:GLN:HG3   | 1.81                     | 0.63              |
| 38:Y:9:LYS:HG2     | 38:Y:55:PRO:HB3   | 1.80                     | 0.63              |
| 38:Y:102:ARG:HG3   | 38:Y:141:ASP:HA   | 1.80                     | 0.63              |
| 51:l:6:LYS:HE3     | 51:l:119:ILE:CG2  | 2.28                     | 0.63              |
| 59:t:8:LEU:N       | 59:t:18:ARG:NH1   | 2.46                     | 0.63              |
| 61:v:88:ASN:OD1    | 61:v:89:VAL:N     | 2.32                     | 0.63              |
| 62:w:33:ILE:CG1    | 62:w:112:TYR:HD1  | 2.11                     | 0.63              |
| 12:AB:118:ILE:HD11 | 12:AB:159:PHE:HA  | 1.81                     | 0.62              |
| 16:C:33:ILE:O      | 21:H:338:GLU:CD   | 2.42                     | 0.62              |
| 17:D:718:A:H5'     | 30:Q:119:ASN:ND2  | 2.13                     | 0.62              |
| 23:J:99:ASP:OD1    | 23:J:100:ASN:N    | 2.31                     | 0.62              |
| 28:O:123:ARG:HG2   | 28:O:123:ARG:O    | 1.99                     | 0.62              |
| 40:a:2682:A:O4'    | 49:j:11:MET:CE    | 2.47                     | 0.62              |
| 40:a:2725:A:C4     | 40:a:2727:A:C8    | 2.87                     | 0.62              |
| 44:e:13:GLU:O      | 44:e:17:GLU:OE1   | 2.16                     | 0.62              |
| 51:l:23:PHE:HB2    | 51:l:111:GLU:OE2  | 1.99                     | 0.62              |
| 5:4:80:HIS:CE1     | 5:4:82:TYR:H      | 2.17                     | 0.62              |
| 8:7:11:U:O2'       | 24:K:33:PHE:CZ    | 2.52                     | 0.62              |
| 9:9:113:PHE:O      | 9:9:123:ILE:HG13  | 1.99                     | 0.62              |
| 24:K:140:THR:O     | 24:K:144:LEU:HD23 | 1.99                     | 0.62              |
| 26:M:66:LEU:HD13   | 26:M:101:MET:HE1  | 1.81                     | 0.62              |
| 29:P:24:GLU:HA     | 29:P:27:GLU:OE1   | 1.98                     | 0.62              |
| 31:R:75:GLN:OE1    | 31:R:75:GLN:N     | 2.32                     | 0.62              |
| 34:U:18:GLN:OE1    | 34:U:37:GLY:O     | 2.17                     | 0.62              |
| 38:Y:60:VAL:HG22   | 38:Y:66:PHE:CB    | 2.23                     | 0.62              |
| 58:s:37:ARG:NH2    | 58:s:44:TYR:OH    | 2.32                     | 0.62              |
| 3:2:56:GLU:OE2     | 3:2:87:LEU:C      | 2.42                     | 0.62              |
| 9:9:23:LEU:HD11    | 9:9:96:PHE:CE2    | 2.34                     | 0.62              |
| 12:AB:141:LEU:O    | 12:AB:151:LYS:C   | 2.42                     | 0.62              |
| 17:D:13:U:O2       | 17:D:914:A:C8     | 2.52                     | 0.62              |
| 20:G:126:PHE:O     | 20:G:126:PHE:CD1  | 2.53                     | 0.62              |
| 21:H:135:LEU:O     | 21:H:169:SER:HA   | 2.00                     | 0.62              |
| 36:W:12:ASP:OD2    | 36:W:35:SER:OG    | 2.14                     | 0.62              |
| 50:k:21:TYR:CE2    | 50:k:38:LYS:HG2   | 2.34                     | 0.62              |
| 64:y:64:ILE:HG13   | 64:y:64:ILE:O     | 1.97                     | 0.62              |
| 8:7:9:U:O4         | 17:D:1196:A:N9    | 2.32                     | 0.62              |
| 9:9:129:LEU:N      | 9:9:130:PRO:HD2   | 2.12                     | 0.62              |
| 11:AA:120:GLN:NE2  | 11:AA:490:GLN:OE1 | 2.32                     | 0.62              |
| 17:D:1228:C:OP1    | 37:X:107:ARG:NH1  | 2.32                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:X:16:VAL:HG12   | 37:X:34:LEU:HD12  | 1.80                     | 0.62              |
| 38:Y:80:LYS:HG3    | 38:Y:86:LYS:O     | 2.00                     | 0.62              |
| 40:a:2315:G:H4'    | 53:n:127:ASN:ND2  | 2.14                     | 0.62              |
| 4:3:68:SER:OG      | 40:a:335:C:O2     | 2.15                     | 0.62              |
| 9:9:50:VAL:HG23    | 38:Y:120:ASP:OD2  | 1.98                     | 0.62              |
| 11:AA:314:ASN:HD21 | 11:AA:348:SER:HA  | 1.62                     | 0.62              |
| 12:AB:141:LEU:HB3  | 12:AB:143:LEU:CD1 | 2.29                     | 0.62              |
| 10:B:31:G:O3'      | 17:D:1340:A:O2'   | 2.17                     | 0.62              |
| 17:D:337:G:H2'     | 17:D:338:A:C8     | 2.34                     | 0.62              |
| 17:D:522:C:OP2     | 31:R:66:TYR:OH    | 2.17                     | 0.62              |
| 17:D:932:C:H5'     | 26:M:4:ARG:HH11   | 1.63                     | 0.62              |
| 20:G:35:ARG:HB3    | 21:H:14:LYS:HZ3   | 1.64                     | 0.62              |
| 21:H:16:ILE:HG22   | 21:H:25:ARG:NH2   | 2.14                     | 0.62              |
| 21:H:19:ARG:O      | 21:H:72:LEU:HB2   | 1.98                     | 0.62              |
| 26:M:4:ARG:CG      | 26:M:5:ARG:CZ     | 2.75                     | 0.62              |
| 40:a:985:C:C2      | 40:a:986:C:C5     | 2.88                     | 0.62              |
| 62:w:37:THR:OG1    | 62:w:40:LYS:HD2   | 2.00                     | 0.62              |
| 12:AB:114:ASP:O    | 12:AB:130:PHE:HB2 | 1.99                     | 0.62              |
| 17:D:562:U:C2'     | 31:R:14:ARG:HH11  | 2.13                     | 0.62              |
| 17:D:1152:A:OP1    | 29:P:70:HIS:ND1   | 2.29                     | 0.62              |
| 53:n:38:MET:SD     | 53:n:150:ARG:HD2  | 2.39                     | 0.62              |
| 6:5:10:DT:C5'      | 11:AA:62:TYR:OH   | 2.48                     | 0.62              |
| 38:Y:99:LYS:NZ     | 38:Y:138:VAL:HG13 | 2.14                     | 0.62              |
| 40:a:1138:G:N3     | 58:s:108:MET:HE2  | 2.14                     | 0.62              |
| 57:r:5:LEU:HD12    | 57:r:17:ASP:O     | 2.00                     | 0.62              |
| 58:s:98:GLU:O      | 58:s:102:GLU:OE1  | 2.18                     | 0.62              |
| 5:4:76:ASP:OD1     | 5:4:77:VAL:N      | 2.33                     | 0.62              |
| 12:AB:102:LYS:HE2  | 14:AE:285:LEU:CB  | 2.29                     | 0.62              |
| 20:G:19:GLN:OE1    | 20:G:21:ARG:HG2   | 2.00                     | 0.62              |
| 26:M:17:LYS:HG3    | 26:M:18:PHE:CD1   | 2.35                     | 0.62              |
| 26:M:18:PHE:HD2    | 26:M:59:LEU:HD21  | 1.65                     | 0.62              |
| 29:P:23:ALA:O      | 29:P:27:GLU:OE1   | 2.18                     | 0.62              |
| 37:X:28:THR:CG2    | 37:X:31:LYS:HE3   | 2.30                     | 0.62              |
| 40:a:1824:G:C3'    | 47:h:52:ARG:HH12  | 2.13                     | 0.62              |
| 46:g:65:ASN:OD1    | 46:g:66:ILE:N     | 2.30                     | 0.62              |
| 61:v:1:MET:HE1     | 61:v:44:ARG:CA    | 2.30                     | 0.62              |
| 6:5:11:DA:H2'      | 12:AB:67:THR:HG21 | 1.82                     | 0.62              |
| 40:a:2307:G:O4'    | 40:a:2308:G:C5    | 2.52                     | 0.62              |
| 62:w:42:LYS:HE2    | 62:w:97:ILE:HG21  | 1.82                     | 0.62              |
| 5:4:77:VAL:HG11    | 5:4:79:ARG:HH21   | 1.64                     | 0.62              |
| 8:7:7:U:H6         | 8:7:7:U:H5''      | 1.64                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:AC:45:ARG:HD3  | 13:AD:38:THR:HB   | 1.82                     | 0.62              |
| 14:AE:87:LYS:HE2  | 29:P:89:ARG:HG2   | 1.82                     | 0.62              |
| 17:D:1157:A:C2    | 17:D:1181:G:C4    | 2.88                     | 0.62              |
| 20:G:49:MET:HE3   | 20:G:199:VAL:O    | 1.99                     | 0.62              |
| 36:W:40:ILE:CD1   | 36:W:66:MET:SD    | 2.77                     | 0.62              |
| 40:a:2682:A:H8    | 49:j:11:MET:HE1   | 1.65                     | 0.62              |
| 54:o:32:ILE:HG13  | 54:o:32:ILE:O     | 2.00                     | 0.62              |
| 17:D:406:G:H21    | 23:J:116:GLN:HE22 | 1.46                     | 0.61              |
| 17:D:1309:G:P     | 37:X:98:ARG:HE    | 2.20                     | 0.61              |
| 24:K:69:ARG:HA    | 24:K:69:ARG:NE    | 2.15                     | 0.61              |
| 38:Y:99:LYS:HZ3   | 38:Y:138:VAL:HG13 | 1.64                     | 0.61              |
| 47:h:141:VAL:HG23 | 47:h:162:VAL:CG1  | 2.30                     | 0.61              |
| 58:s:11:VAL:HG11  | 58:s:13:ARG:NH1   | 2.15                     | 0.61              |
| 62:w:47:VAL:O     | 62:w:51:LEU:HD23  | 2.00                     | 0.61              |
| 6:5:9:DG:P        | 11:AA:473:ARG:CG  | 2.88                     | 0.61              |
| 9:9:52:MET:C      | 9:9:52:MET:HE3    | 2.25                     | 0.61              |
| 10:A:5:G:H2'      | 10:A:6:G:H5'      | 1.82                     | 0.61              |
| 11:AA:528:ARG:NH2 | 11:AA:576:SER:O   | 2.30                     | 0.61              |
| 18:E:81:ALA:C     | 18:E:85:LYS:HZ3   | 2.07                     | 0.61              |
| 21:H:61:GLU:HG2   | 21:H:62:ILE:HG23  | 1.81                     | 0.61              |
| 22:I:58:GLU:OE2   | 29:P:94:ALA:CB    | 2.48                     | 0.61              |
| 32:S:19:LYS:HG3   | 32:S:20:TYR:CE1   | 2.35                     | 0.61              |
| 38:Y:102:ARG:HA   | 38:Y:102:ARG:HE   | 1.63                     | 0.61              |
| 40:a:1839:G:C8    | 40:a:1927:A:H1'   | 2.35                     | 0.61              |
| 6:5:10:DT:H1'     | 12:AB:71:ALA:H    | 0.83                     | 0.61              |
| 20:G:30:PHE:CD1   | 20:G:201:PRO:CG   | 2.83                     | 0.61              |
| 27:N:43:GLU:CD    | 27:N:101:ILE:HG21 | 2.25                     | 0.61              |
| 37:X:22:ILE:HB    | 37:X:25:VAL:HG12  | 1.80                     | 0.61              |
| 38:Y:79:LEU:CD1   | 38:Y:132:ALA:HA   | 2.29                     | 0.61              |
| 40:a:1406:U:C2    | 40:a:1407:G:C8    | 2.88                     | 0.61              |
| 49:j:1:MET:HE2    | 49:j:100:LEU:HD11 | 1.82                     | 0.61              |
| 2:1:98:LYS:NZ     | 40:a:2011:U:O3'   | 2.34                     | 0.61              |
| 5:4:77:VAL:HG22   | 5:4:79:ARG:HE     | 1.64                     | 0.61              |
| 6:5:11:DA:C2'     | 12:AB:67:THR:CG2  | 2.77                     | 0.61              |
| 11:AA:472:GLU:HG3 | 11:AA:473:ARG:HD3 | 1.83                     | 0.61              |
| 12:AB:35:LEU:HB3  | 12:AB:37:LYS:HD3  | 1.82                     | 0.61              |
| 10:B:5:G:H2'      | 10:B:6:G:H5'      | 1.83                     | 0.61              |
| 17:D:563:A:C2     | 17:D:567:G:C5     | 2.89                     | 0.61              |
| 3:2:56:GLU:OE2    | 3:2:87:LEU:O      | 2.18                     | 0.61              |
| 8:7:11:U:O4'      | 24:K:20:ARG:NH2   | 2.32                     | 0.61              |
| 12:AB:102:LYS:CD  | 14:AE:285:LEU:HA  | 2.31                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:AE:74:LYS:HZ3  | 29:P:89:ARG:HB3   | 1.63                     | 0.61              |
| 28:O:94:LEU:HB3   | 28:O:97:GLU:OE2   | 2.00                     | 0.61              |
| 30:Q:84:VAL:HG23  | 30:Q:107:ILE:CD1  | 2.30                     | 0.61              |
| 40:a:1277:G:N3    | 62:w:23:ASN:ND2   | 2.47                     | 0.61              |
| 50:k:34:LEU:HB3   | 50:k:51:GLU:HG3   | 1.82                     | 0.61              |
| 57:r:114:GLU:OE2  | 57:r:134:VAL:N    | 2.33                     | 0.61              |
| 17:D:1124:G:O2'   | 17:D:1145:A:N6    | 2.33                     | 0.61              |
| 20:G:110:SER:HA   | 20:G:113:ARG:HE   | 1.65                     | 0.61              |
| 21:H:135:LEU:CB   | 21:H:167:VAL:CB   | 2.78                     | 0.61              |
| 24:K:81:LEU:HG    | 24:K:96:MET:HE1   | 1.83                     | 0.61              |
| 26:M:103:TRP:O    | 26:M:106:GLU:HG3  | 2.01                     | 0.61              |
| 29:P:26:VAL:HG12  | 29:P:30:LYS:NZ    | 2.16                     | 0.61              |
| 33:T:67:LEU:HD12  | 33:T:78:TYR:CE1   | 2.35                     | 0.61              |
| 38:Y:91:LYS:HZ1   | 38:Y:97:VAL:HG21  | 1.65                     | 0.61              |
| 40:a:754:U:H2'    | 40:a:755:U:C6     | 2.34                     | 0.61              |
| 50:k:34:LEU:HB3   | 50:k:51:GLU:CG    | 2.31                     | 0.61              |
| 54:o:13:ARG:HD3   | 60:u:58:TYR:O     | 2.00                     | 0.61              |
| 6:5:10:DT:H73     | 11:AA:62:TYR:CG   | 2.18                     | 0.61              |
| 12:AB:140:MET:HA  | 12:AB:153:SER:HA  | 1.83                     | 0.61              |
| 17:D:687:A:C2     | 17:D:704:A:C5     | 2.88                     | 0.61              |
| 17:D:1006:G:H2'   | 17:D:1007:U:C6    | 2.36                     | 0.61              |
| 38:Y:9:LYS:HE2    | 38:Y:55:PRO:HG3   | 1.82                     | 0.61              |
| 6:5:10:DT:C4      | 11:AA:62:TYR:HD2  | 2.12                     | 0.61              |
| 9:9:23:LEU:HA     | 9:9:118:ILE:CG1   | 2.31                     | 0.61              |
| 10:A:33:U:O3'     | 26:M:84:THR:OG1   | 2.16                     | 0.61              |
| 16:C:60:LYS:NZ    | 17:D:734:G:C2'    | 2.64                     | 0.61              |
| 36:W:67:VAL:HG21  | 46:g:57:VAL:HG22  | 1.82                     | 0.61              |
| 46:g:1:MET:HE2    | 46:g:6:HIS:CD2    | 2.35                     | 0.61              |
| 60:u:84:LYS:NZ    | 60:u:98:ALA:O     | 2.20                     | 0.61              |
| 61:v:111:GLU:HA   | 61:v:114:ARG:HE   | 1.66                     | 0.61              |
| 1:0:73:LYS:NZ     | 40:a:1225:G:OP1   | 2.34                     | 0.61              |
| 11:AA:55:SER:OG   | 11:AA:465:ARG:NH1 | 2.33                     | 0.61              |
| 10:B:36:U:H2'     | 10:B:37:A:C8      | 2.35                     | 0.61              |
| 16:C:45:THR:HA    | 21:H:340:ARG:NH2  | 2.15                     | 0.61              |
| 20:G:38:VAL:CG2   | 21:H:75:VAL:HG21  | 2.30                     | 0.61              |
| 25:L:102:MET:HG2  | 25:L:103:VAL:N    | 2.06                     | 0.61              |
| 47:h:164:ILE:HG23 | 47:h:164:ILE:O    | 2.01                     | 0.61              |
| 58:s:13:ARG:HH22  | 58:s:50:THR:CA    | 2.14                     | 0.61              |
| 65:z:74:ILE:HD13  | 65:z:79:PHE:CD1   | 2.34                     | 0.61              |
| 9:9:61:ARG:NE     | 40:a:1046:A:O5'   | 2.34                     | 0.61              |
| 14:AE:785:ASP:O   | 14:AE:789:LYS:HB2 | 2.01                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:AE:888:CYS:SG   | 14:AE:889:ASP:N    | 2.74                     | 0.61              |
| 10:B:65:C:H2'      | 10:B:66:C:H5'      | 1.83                     | 0.61              |
| 20:G:114:LEU:HD13  | 20:G:144:LEU:HB2   | 1.83                     | 0.61              |
| 32:S:87:ALA:HA     | 32:S:90:ARG:NH1    | 2.15                     | 0.61              |
| 35:V:60:GLU:OE1    | 35:V:76:VAL:HG23   | 2.01                     | 0.61              |
| 36:W:45:ILE:HA     | 36:W:62:VAL:CG1    | 2.31                     | 0.61              |
| 9:9:47:GLU:HA      | 9:9:94:ARG:HH22    | 1.65                     | 0.60              |
| 10:A:65:C:H2'      | 10:A:66:C:H5'      | 1.83                     | 0.60              |
| 27:N:24:ALA:HB1    | 27:N:60:GLU:OE2    | 2.00                     | 0.60              |
| 28:O:55:VAL:O      | 28:O:57:MET:N      | 2.34                     | 0.60              |
| 39:Z:8:ILE:HG13    | 39:Z:9:GLU:N       | 2.15                     | 0.60              |
| 9:9:14:GLU:OE1     | 9:9:62:ARG:O       | 2.19                     | 0.60              |
| 14:AE:1275:LEU:HB3 | 14:AE:1278:GLU:HB2 | 1.83                     | 0.60              |
| 20:G:73:LYS:O      | 20:G:74:ARG:HG2    | 2.00                     | 0.60              |
| 22:I:14:ILE:HG22   | 22:I:15:VAL:HG13   | 1.82                     | 0.60              |
| 22:I:45:LYS:NZ     | 22:I:46:GLU:OE1    | 2.29                     | 0.60              |
| 35:V:61:ILE:HG13   | 35:V:73:TRP:CZ3    | 2.36                     | 0.60              |
| 53:n:122:PHE:CZ    | 53:n:170:LEU:HD12  | 2.36                     | 0.60              |
| 9:9:25:ALA:HB2     | 9:9:96:PHE:CD1     | 2.36                     | 0.60              |
| 27:N:88:ARG:HB2    | 27:N:91:GLU:OE1    | 2.00                     | 0.60              |
| 28:O:57:MET:HA     | 28:O:60:LYS:HE2    | 1.83                     | 0.60              |
| 38:Y:36:GLU:HG3    | 38:Y:66:PHE:CE1    | 2.36                     | 0.60              |
| 40:a:413:C:H2'     | 40:a:414:C:H6      | 1.66                     | 0.60              |
| 40:a:753:A:C2      | 40:a:754:U:C6      | 2.89                     | 0.60              |
| 61:v:75:GLU:HG3    | 61:v:90:GLU:OE1    | 2.01                     | 0.60              |
| 11:AA:1072:ASN:ND2 | 11:AA:1111:GLN:OE1 | 2.34                     | 0.60              |
| 14:AE:86:GLU:OE1   | 14:AE:86:GLU:N     | 2.34                     | 0.60              |
| 14:AE:741:ALA:O    | 14:AE:762:ASN:ND2  | 2.32                     | 0.60              |
| 34:U:5:ARG:HH22    | 34:U:24:SER:HA     | 1.66                     | 0.60              |
| 38:Y:19:PRO:O      | 38:Y:24:GLY:CA     | 2.48                     | 0.60              |
| 40:a:271:G:C4      | 40:a:272:A:C8      | 2.89                     | 0.60              |
| 40:a:372:G:O2'     | 40:a:400:G:O6      | 2.16                     | 0.60              |
| 40:a:1070:A:N7     | 40:a:1096:A:O2'    | 2.35                     | 0.60              |
| 45:f:40:ASP:C      | 45:f:45:ARG:NH2    | 2.60                     | 0.60              |
| 47:h:84:ASP:HB2    | 47:h:91:ILE:HD12   | 1.84                     | 0.60              |
| 60:u:51:GLU:OE1    | 60:u:51:GLU:N      | 2.34                     | 0.60              |
| 2:1:31:GLN:OE1     | 2:1:31:GLN:N       | 2.28                     | 0.60              |
| 12:AB:31:PRO:O     | 12:AB:50:LEU:N     | 2.31                     | 0.60              |
| 18:E:28:MET:SD     | 18:E:57:ILE:HG22   | 2.42                     | 0.60              |
| 24:K:159:LYS:NZ    | 27:N:44:GLY:HA3    | 2.16                     | 0.60              |
| 26:M:137:LYS:O     | 26:M:141:VAL:HG23  | 2.01                     | 0.60              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 28:O:56:ASP:O    | 28:O:57:MET:HE2    | 2.02                     | 0.60              |
| 38:Y:72:THR:OG1  | 38:Y:73:PRO:HD2    | 2.01                     | 0.60              |
| 43:d:42:C:P      | 53:n:64:LYS:HZ1    | 2.24                     | 0.60              |
| 61:v:38:ARG:HA   | 61:v:96:ILE:O      | 2.00                     | 0.60              |
| 6:5:9:DG:O5'     | 11:AA:473:ARG:CB   | 2.49                     | 0.60              |
| 9:9:50:VAL:CG2   | 38:Y:119:ALA:HB3   | 2.20                     | 0.60              |
| 17:D:652:U:H4'   | 27:N:56:LYS:NZ     | 2.17                     | 0.60              |
| 19:F:49:LYS:O    | 19:F:53:VAL:HG23   | 2.02                     | 0.60              |
| 26:M:50:LEU:HD21 | 26:M:121:ALA:CA    | 2.28                     | 0.60              |
| 53:n:25:VAL:O    | 53:n:28:VAL:HG12   | 2.02                     | 0.60              |
| 53:n:38:MET:HG3  | 53:n:57:LEU:HD21   | 1.83                     | 0.60              |
| 58:s:13:ARG:NH2  | 58:s:49:ASP:O      | 2.34                     | 0.60              |
| 1:0:51:VAL:O     | 1:0:51:VAL:HG13    | 2.02                     | 0.60              |
| 12:AB:90:SER:HB3 | 12:AB:93:ILE:HB    | 1.84                     | 0.60              |
| 12:AB:92:VAL:HA  | 12:AB:96:LEU:HB2   | 1.83                     | 0.60              |
| 12:AB:129:ILE:HB | 12:AB:142:LEU:HD22 | 1.83                     | 0.60              |
| 17:D:718:A:O2'   | 19:F:34:ARG:NH2    | 2.34                     | 0.60              |
| 17:D:1160:G:C2   | 17:D:1161:C:C6     | 2.89                     | 0.60              |
| 24:K:112:ARG:O   | 24:K:116:GLU:OE1   | 2.19                     | 0.60              |
| 24:K:113:ALA:HA  | 24:K:116:GLU:OE1   | 2.00                     | 0.60              |
| 25:L:42:TRP:CZ2  | 25:L:102:MET:HG3   | 2.36                     | 0.60              |
| 35:V:10:GLY:HA3  | 35:V:25:ILE:HD13   | 1.83                     | 0.60              |
| 40:a:1257:C:H4'  | 51:l:78:TRP:CD2    | 2.37                     | 0.60              |
| 48:i:22:LEU:HG   | 48:i:23:THR:N      | 2.17                     | 0.60              |
| 59:t:8:LEU:N     | 59:t:18:ARG:HH12   | 1.98                     | 0.60              |
| 2:1:1:MET:SD     | 2:1:3:THR:OG1      | 2.59                     | 0.60              |
| 7:6:25:DT:H2'    | 11:AA:496:LYS:CE   | 2.28                     | 0.60              |
| 9:9:23:LEU:HD21  | 9:9:96:PHE:CG      | 2.36                     | 0.60              |
| 12:AB:82:GLY:HA2 | 14:AE:142:GLU:OE1  | 2.01                     | 0.60              |
| 14:AE:64:PRO:HG3 | 14:AE:90:VAL:HG12  | 1.83                     | 0.60              |
| 25:L:9:MET:HE2   | 25:L:51:ILE:HD11   | 1.83                     | 0.60              |
| 27:N:106:THR:HB  | 27:N:121:LEU:HD13  | 1.83                     | 0.60              |
| 29:P:25:ILE:O    | 29:P:28:THR:OG1    | 2.19                     | 0.60              |
| 34:U:76:LYS:C    | 34:U:80:LYS:HZ3    | 2.10                     | 0.60              |
| 39:Z:14:MET:HG3  | 39:Z:15:SER:N      | 2.17                     | 0.60              |
| 40:a:548:G:H3'   | 40:a:549:G:O4'     | 2.01                     | 0.60              |
| 40:a:2191:A:H2'  | 40:a:2192:U:C6     | 2.36                     | 0.60              |
| 46:g:5:ILE:HD12  | 53:n:64:LYS:CE     | 2.31                     | 0.60              |
| 58:s:73:VAL:HG13 | 58:s:86:GLN:HG2    | 1.84                     | 0.60              |
| 65:z:74:ILE:HD11 | 65:z:79:PHE:CA     | 2.30                     | 0.60              |
| 6:5:11:DA:H2'    | 12:AB:67:THR:CG2   | 2.32                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:9:47:GLU:HG3     | 9:9:94:ARG:NH1     | 2.16                     | 0.60              |
| 9:9:98:GLU:HA      | 9:9:101:LYS:HG2    | 1.83                     | 0.60              |
| 9:9:123:ILE:O      | 9:9:123:ILE:HG23   | 2.02                     | 0.60              |
| 11:AA:69:GLN:HE21  | 11:AA:101:ARG:HD2  | 1.67                     | 0.60              |
| 12:AB:142:LEU:HA   | 12:AB:151:LYS:HA   | 1.83                     | 0.60              |
| 13:AD:112:ALA:HB3  | 13:AD:126:PRO:HA   | 1.83                     | 0.60              |
| 14:AE:814:CYS:SG   | 14:AE:883:ARG:NH2  | 2.74                     | 0.60              |
| 17:D:1169:A:H2'    | 17:D:1170:A:C8     | 2.37                     | 0.60              |
| 40:a:563:A:OP1     | 65:z:41:LYS:NZ     | 2.35                     | 0.60              |
| 40:a:639:U:H2'     | 40:a:640:C:C6      | 2.36                     | 0.60              |
| 40:a:2363:G:OP2    | 54:o:40:ARG:HD2    | 2.01                     | 0.60              |
| 54:o:30:ARG:HH12   | 60:u:62:PRO:CA     | 2.14                     | 0.60              |
| 61:v:77:PRO:HG2    | 61:v:80:VAL:CG2    | 2.31                     | 0.60              |
| 1:0:68:ARG:HH12    | 40:a:1223:G:P      | 2.25                     | 0.60              |
| 3:2:56:GLU:OE1     | 3:2:86:THR:O       | 2.19                     | 0.60              |
| 9:9:7:ASP:OD1      | 9:9:8:LYS:N        | 2.35                     | 0.60              |
| 10:A:36:U:H2'      | 10:A:37:A:C8       | 2.35                     | 0.60              |
| 17:D:496:A:N3      | 17:D:496:A:H2'     | 2.17                     | 0.60              |
| 17:D:1290:G:H4'    | 26:M:35:LYS:HZ3    | 1.66                     | 0.60              |
| 24:K:45:ARG:HB3    | 24:K:71:MET:HE2    | 1.82                     | 0.60              |
| 26:M:111:ARG:O     | 26:M:119:ARG:NH1   | 2.34                     | 0.60              |
| 27:N:104:VAL:HG23  | 27:N:125:ILE:HD13  | 1.83                     | 0.60              |
| 37:X:55:THR:O      | 37:X:59:GLU:OE1    | 2.18                     | 0.60              |
| 40:a:575:A:C2      | 40:a:576:U:C5      | 2.90                     | 0.60              |
| 45:f:41:THR:O      | 45:f:44:ILE:N      | 2.30                     | 0.60              |
| 47:h:67:PHE:CE1    | 47:h:156:ARG:HD2   | 2.37                     | 0.60              |
| 58:s:102:GLU:HB3   | 58:s:119:PHE:HZ    | 1.66                     | 0.60              |
| 60:u:76:GLU:HG3    | 60:u:111:ILE:CD1   | 2.31                     | 0.60              |
| 7:6:25:DT:OP1      | 11:AA:496:LYS:C    | 2.43                     | 0.59              |
| 8:7:9:U:O4         | 17:D:1196:A:C8     | 2.55                     | 0.59              |
| 12:AB:89:PRO:CG    | 14:AE:290:ILE:CG2  | 2.79                     | 0.59              |
| 12:AB:140:MET:HB3  | 12:AB:150:ILE:HD12 | 1.84                     | 0.59              |
| 13:AD:211:ILE:HG12 | 13:AD:219:ARG:HH12 | 1.65                     | 0.59              |
| 17:D:1290:G:H4'    | 26:M:35:LYS:NZ     | 2.17                     | 0.59              |
| 23:J:62:ARG:HG2    | 23:J:72:PHE:CE1    | 2.37                     | 0.59              |
| 40:a:2298:A:C4     | 40:a:2321:U:C5     | 2.90                     | 0.59              |
| 40:a:2780:G:P      | 58:s:120:ARG:NH1   | 2.74                     | 0.59              |
| 47:h:30:PHE:O      | 47:h:34:LEU:HD23   | 2.02                     | 0.59              |
| 49:j:25:THR:HG21   | 49:j:193:VAL:HG22  | 1.84                     | 0.59              |
| 58:s:55:ILE:HG13   | 58:s:123:LYS:NZ    | 2.17                     | 0.59              |
| 59:t:5:GLN:HA      | 59:t:20:MET:CE     | 2.32                     | 0.59              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 62:w:33:ILE:CG1     | 62:w:112:TYR:CD1   | 2.85                     | 0.59              |
| 62:w:60:VAL:HA      | 62:w:63:ARG:NH1    | 2.17                     | 0.59              |
| 9:9:97:LYS:NZ       | 9:9:130:PRO:HA     | 2.17                     | 0.59              |
| 17:D:1439:G:P       | 18:E:33:LYS:HZ1    | 2.23                     | 0.59              |
| 29:P:86:ALA:C       | 29:P:90:LEU:HD13   | 2.27                     | 0.59              |
| 38:Y:5:GLN:CG       | 38:Y:61:TYR:CE1    | 2.76                     | 0.59              |
| 40:a:1432:G:H2'     | 40:a:1433:A:C8     | 2.37                     | 0.59              |
| 12:AB:117:ILE:O     | 12:AB:160:ARG:O    | 2.20                     | 0.59              |
| 14:AE:1221:LEU:HD22 | 14:AE:1306:LEU:HB2 | 1.85                     | 0.59              |
| 17:D:13:U:N3        | 17:D:915:A:N6      | 2.51                     | 0.59              |
| 17:D:1125:U:C2      | 17:D:1127:G:C8     | 2.89                     | 0.59              |
| 27:N:47:GLU:OE2     | 27:N:64:LYS:HA     | 2.02                     | 0.59              |
| 31:R:7:LEU:CD2      | 31:R:12:ARG:NH2    | 2.65                     | 0.59              |
| 38:Y:23:VAL:HG23    | 38:Y:24:GLY:N      | 2.17                     | 0.59              |
| 38:Y:126:ARG:HH22   | 40:a:1083:U:P      | 2.25                     | 0.59              |
| 40:a:323:C:H2'      | 51:l:163:ASN:OD1   | 2.02                     | 0.59              |
| 40:a:2189:U:P       | 40:a:2189:U:O4'    | 2.60                     | 0.59              |
| 51:l:1:MET:CE       | 51:l:16:GLU:HA     | 2.26                     | 0.59              |
| 53:n:122:PHE:O      | 53:n:123:ASP:OD1   | 2.19                     | 0.59              |
| 59:t:8:LEU:CA       | 59:t:18:ARG:HH12   | 2.15                     | 0.59              |
| 14:AE:92:VAL:HG22   | 14:AE:92:VAL:O     | 2.01                     | 0.59              |
| 14:AE:1161:GLY:HA3  | 14:AE:1179:PRO:HA  | 1.83                     | 0.59              |
| 17:D:657:U:C4'      | 33:T:28:GLN:HE22   | 2.16                     | 0.59              |
| 17:D:890:G:O2'      | 17:D:906:A:N6      | 2.35                     | 0.59              |
| 17:D:978:A:C5       | 17:D:1319:A:C2     | 2.90                     | 0.59              |
| 23:J:74:ASN:HA      | 23:J:77:LYS:NZ     | 2.17                     | 0.59              |
| 32:S:20:TYR:HD2     | 32:S:55:SER:OG     | 1.85                     | 0.59              |
| 40:a:1172:C:H2'     | 40:a:1173:U:O4'    | 2.02                     | 0.59              |
| 50:k:19:HIS:ND1     | 50:k:41:PRO:CD     | 2.65                     | 0.59              |
| 9:9:54:VAL:HG13     | 9:9:54:VAL:O       | 2.03                     | 0.59              |
| 10:A:69:C:H2'       | 10:A:70:G:O4'      | 2.02                     | 0.59              |
| 10:B:69:C:H2'       | 10:B:70:G:O4'      | 2.02                     | 0.59              |
| 17:D:718:A:C4       | 30:Q:118:HIS:ND1   | 2.71                     | 0.59              |
| 17:D:921:U:H4'      | 24:K:23:LYS:NZ     | 2.18                     | 0.59              |
| 20:G:23:TRP:HZ3     | 20:G:25:PRO:HA     | 1.67                     | 0.59              |
| 21:H:81:GLU:O       | 21:H:82:THR:HG23   | 2.02                     | 0.59              |
| 21:H:333:LEU:O      | 21:H:334:ASP:OD1   | 2.19                     | 0.59              |
| 22:I:54:ARG:NH2     | 22:I:56:VAL:HG21   | 2.18                     | 0.59              |
| 37:X:81:MET:HE1     | 37:X:92:ARG:HD3    | 1.83                     | 0.59              |
| 40:a:468:G:N7       | 52:m:39:ARG:NH2    | 2.42                     | 0.59              |
| 40:a:947:A:H2'      | 40:a:948:C:C6      | 2.37                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:a:1322:A:C5     | 40:a:1323:C:C5    | 2.90                     | 0.59              |
| 40:a:1798:U:OP2    | 47:h:271:ARG:NH2  | 2.36                     | 0.59              |
| 40:a:2460:U:C2     | 40:a:2461:A:C8    | 2.91                     | 0.59              |
| 44:e:2:LYS:CE      | 44:e:52:ARG:HE    | 2.15                     | 0.59              |
| 64:y:7:GLN:CD      | 64:y:7:GLN:C      | 2.71                     | 0.59              |
| 65:z:74:ILE:CD1    | 65:z:74:ILE:CB    | 2.76                     | 0.59              |
| 6:5:10:DT:N1       | 11:AA:62:TYR:CE2  | 2.65                     | 0.59              |
| 12:AB:99:TYR:O     | 12:AB:100:LYS:HG2 | 2.03                     | 0.59              |
| 17:D:736:C:O2'     | 25:L:88:MET:HE1   | 2.02                     | 0.59              |
| 17:D:1055:A:C2'    | 22:I:156:ARG:HH21 | 2.15                     | 0.59              |
| 23:J:91:LEU:HD21   | 23:J:195:ILE:HD12 | 1.84                     | 0.59              |
| 24:K:16:ILE:HD11   | 24:K:38:VAL:HG12  | 1.83                     | 0.59              |
| 26:M:18:PHE:HB3    | 26:M:59:LEU:HD11  | 1.84                     | 0.59              |
| 53:n:4:LEU:HD11    | 53:n:101:GLU:HA   | 1.84                     | 0.59              |
| 2:1:86:MET:CE      | 2:1:88:ARG:HD3    | 2.32                     | 0.59              |
| 9:9:17:GLU:HG2     | 9:9:88:HIS:NE2    | 2.18                     | 0.59              |
| 9:9:33:VAL:HG22    | 9:9:36:ASP:CG     | 2.27                     | 0.59              |
| 9:9:46:ARG:CG      | 9:9:94:ARG:HH21   | 2.02                     | 0.59              |
| 9:9:60:LEU:HA      | 9:9:64:VAL:HB     | 1.84                     | 0.59              |
| 10:A:70:G:H2'      | 10:A:71:C:H5''    | 1.85                     | 0.59              |
| 16:C:29:LEU:HD23   | 16:C:59:ILE:HD13  | 1.83                     | 0.59              |
| 20:G:26:LYS:CD     | 20:G:193:PRO:HG2  | 2.32                     | 0.59              |
| 20:G:128:LYS:HD2   | 20:G:128:LYS:O    | 2.03                     | 0.59              |
| 37:X:25:VAL:HG23   | 37:X:29:ARG:CB    | 2.32                     | 0.59              |
| 37:X:25:VAL:HG23   | 37:X:29:ARG:HB2   | 1.85                     | 0.59              |
| 40:a:856:G:H2'     | 40:a:857:G:C8     | 2.37                     | 0.59              |
| 40:a:1277:G:H5'    | 62:w:20:MET:HE2   | 1.84                     | 0.59              |
| 60:u:76:GLU:HG3    | 60:u:111:ILE:HD13 | 1.84                     | 0.59              |
| 16:C:73:ARG:NH1    | 30:Q:113:VAL:HA   | 2.18                     | 0.59              |
| 17:D:878:A:OP2     | 27:N:80:ARG:NH1   | 2.35                     | 0.59              |
| 27:N:43:GLU:HG2    | 27:N:101:ILE:HD13 | 1.84                     | 0.59              |
| 40:a:2682:A:H8     | 49:j:11:MET:CE    | 2.15                     | 0.59              |
| 40:a:2815:C:C2     | 40:a:2816:G:C8    | 2.91                     | 0.59              |
| 50:k:35:GLU:OE2    | 50:k:48:ILE:HG23  | 2.03                     | 0.59              |
| 55:p:85:LYS:NZ     | 55:p:164:TYR:HD1  | 2.01                     | 0.59              |
| 57:r:68:ARG:O      | 57:r:72:ILE:HD12  | 2.03                     | 0.59              |
| 1:0:61:ALA:HB1     | 1:0:96:VAL:HG22   | 1.84                     | 0.59              |
| 8:7:18:U:C6        | 8:7:18:U:C5'      | 2.85                     | 0.59              |
| 9:9:103:ASN:HA     | 9:9:107:GLU:OE2   | 2.02                     | 0.59              |
| 11:AA:1142:ARG:NH1 | 11:AA:1161:LEU:O  | 2.36                     | 0.59              |
| 18:E:32:ILE:HG12   | 18:E:75:HIS:CE1   | 2.37                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:H:273:ARG:CZ   | 21:H:297:GLU:HG3   | 2.33                     | 0.59              |
| 24:K:12:GLN:HB3   | 24:K:14:LYS:NZ     | 2.18                     | 0.59              |
| 32:S:42:TRP:CH2   | 46:g:66:ILE:HA     | 2.38                     | 0.59              |
| 38:Y:5:GLN:HE22   | 38:Y:60:VAL:C      | 2.10                     | 0.59              |
| 38:Y:33:ASN:HB3   | 38:Y:36:GLU:CG     | 2.30                     | 0.59              |
| 38:Y:70:THR:O     | 38:Y:71:LYS:HG3    | 2.03                     | 0.59              |
| 40:a:654:A:H61    | 54:o:19:LYS:HD2    | 1.68                     | 0.59              |
| 40:a:1817:G:H3'   | 47:h:156:ARG:HH22  | 1.67                     | 0.59              |
| 40:a:2225:A:H4'   | 40:a:2226:C:O5'    | 2.03                     | 0.59              |
| 53:n:46:ASP:OD1   | 53:n:49:LEU:HD13   | 2.03                     | 0.59              |
| 58:s:102:GLU:CD   | 58:s:124:VAL:HG11  | 2.28                     | 0.59              |
| 59:t:88:ASN:ND2   | 59:t:90:ASN:OD1    | 2.36                     | 0.59              |
| 8:7:9:U:O4        | 17:D:1196:A:O4'    | 2.21                     | 0.59              |
| 11:AA:371:ARG:NH1 | 12:AB:67:THR:OG1   | 2.34                     | 0.59              |
| 12:AB:158:GLU:HB3 | 12:AB:162:LEU:HD22 | 1.85                     | 0.59              |
| 16:C:14:THR:HG21  | 16:C:48:ARG:NE     | 2.17                     | 0.59              |
| 16:C:51:TYR:HD1   | 16:C:54:GLN:NE2    | 2.00                     | 0.59              |
| 20:G:35:ARG:HD2   | 21:H:14:LYS:HE3    | 1.84                     | 0.59              |
| 21:H:131:LEU:CB   | 21:H:167:VAL:HA    | 2.32                     | 0.59              |
| 21:H:291:GLY:HA2  | 21:H:305:HIS:HA    | 1.85                     | 0.59              |
| 22:I:142:MET:HE2  | 22:I:149:ILE:HG22  | 1.83                     | 0.59              |
| 26:M:50:LEU:HD11  | 26:M:124:LEU:HB2   | 1.85                     | 0.59              |
| 30:Q:20:VAL:CG1   | 30:Q:85:MET:HE1    | 2.33                     | 0.59              |
| 30:Q:51:GLY:O     | 30:Q:56:ARG:CZ     | 2.51                     | 0.59              |
| 33:T:60:VAL:O     | 33:T:64:ARG:HG2    | 2.03                     | 0.59              |
| 33:T:64:ARG:CZ    | 33:T:64:ARG:HB3    | 2.32                     | 0.59              |
| 38:Y:99:LYS:HD3   | 38:Y:138:VAL:O     | 2.02                     | 0.59              |
| 39:Z:8:ILE:HG13   | 39:Z:9:GLU:H       | 1.68                     | 0.59              |
| 40:a:567:U:OP2    | 60:u:29:LYS:NZ     | 2.35                     | 0.59              |
| 40:a:685:A:O2'    | 40:a:773:U:O4      | 2.17                     | 0.59              |
| 40:a:993:G:OP2    | 65:z:51:ARG:NH2    | 2.36                     | 0.59              |
| 52:m:1:MET:HE3    | 52:m:3:ARG:HH11    | 1.67                     | 0.59              |
| 7:6:20:DA:C6      | 8:7:33:G:C2        | 2.91                     | 0.58              |
| 8:7:15:U:OP1      | 22:I:132:ARG:NH2   | 2.35                     | 0.58              |
| 11:AA:707:ALA:O   | 11:AA:711:ASP:HB2  | 2.03                     | 0.58              |
| 16:C:12:ARG:CG    | 21:H:264:GLU:CB    | 2.81                     | 0.58              |
| 16:C:73:ARG:HH12  | 30:Q:113:VAL:CA    | 2.16                     | 0.58              |
| 20:G:96:TRP:CH2   | 20:G:100:MET:HE3   | 2.38                     | 0.58              |
| 24:K:93:ARG:HB3   | 24:K:93:ARG:NH2    | 2.18                     | 0.58              |
| 33:T:11:ILE:HG21  | 33:T:31:LEU:HD13   | 1.85                     | 0.58              |
| 35:V:11:ARG:HE    | 35:V:58:VAL:CG2    | 2.16                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:a:15:G:O2'     | 48:i:15:MET:CE    | 2.51                     | 0.58              |
| 51:l:62:GLN:O     | 51:l:69:ARG:HD3   | 2.03                     | 0.58              |
| 51:l:119:ILE:O    | 51:l:187:VAL:HA   | 2.03                     | 0.58              |
| 3:2:56:GLU:OE1    | 3:2:56:GLU:N      | 2.33                     | 0.58              |
| 9:9:94:ARG:CB     | 9:9:97:LYS:HE2    | 2.32                     | 0.58              |
| 12:AB:19:GLU:O    | 12:AB:23:ARG:HB2  | 2.03                     | 0.58              |
| 12:AB:126:PHE:CE1 | 14:AE:87:LYS:HD3  | 2.38                     | 0.58              |
| 16:C:73:ARG:CZ    | 30:Q:113:VAL:HG12 | 2.32                     | 0.58              |
| 20:G:106:THR:HA   | 20:G:109:GLN:NE2  | 2.18                     | 0.58              |
| 24:K:148:ASN:OD1  | 27:N:96:MET:HE1   | 2.03                     | 0.58              |
| 37:X:22:ILE:HG23  | 37:X:66:GLU:OE2   | 2.03                     | 0.58              |
| 38:Y:56:VAL:HA    | 38:Y:71:LYS:NZ    | 2.08                     | 0.58              |
| 38:Y:109:ALA:HB2  | 38:Y:128:ILE:HG13 | 1.85                     | 0.58              |
| 40:a:2335:A:OP2   | 63:x:13:ARG:CD    | 2.51                     | 0.58              |
| 3:2:56:GLU:OE1    | 3:2:87:LEU:C      | 2.46                     | 0.58              |
| 5:4:63:ILE:HD11   | 5:4:91:PHE:CE2    | 2.37                     | 0.58              |
| 9:9:78:GLY:N      | 9:9:79:PRO:CD     | 2.65                     | 0.58              |
| 10:B:15:G:N1      | 10:B:20:U:O2      | 2.36                     | 0.58              |
| 17:D:736:C:H5''   | 25:L:90:MET:HE2   | 1.84                     | 0.58              |
| 21:H:155:LYS:O    | 21:H:169:SER:N    | 2.35                     | 0.58              |
| 34:U:19:VAL:HG12  | 34:U:37:GLY:C     | 2.28                     | 0.58              |
| 37:X:93:ARG:HG2   | 37:X:95:LEU:HD23  | 1.84                     | 0.58              |
| 40:a:70:G:H4'     | 40:a:71:A:OP1     | 2.03                     | 0.58              |
| 40:a:1197:G:H2'   | 40:a:1198:U:H6    | 1.68                     | 0.58              |
| 40:a:1406:U:O2'   | 40:a:1407:G:O4'   | 2.20                     | 0.58              |
| 40:a:2243:U:H2'   | 40:a:2244:U:C6    | 2.38                     | 0.58              |
| 47:h:62:TYR:CE2   | 47:h:64:ILE:HD13  | 2.38                     | 0.58              |
| 47:h:181:MET:HE2  | 47:h:181:MET:N    | 2.18                     | 0.58              |
| 50:k:7:GLU:CD     | 50:k:7:GLU:H      | 2.11                     | 0.58              |
| 53:n:4:LEU:HD11   | 53:n:101:GLU:N    | 2.18                     | 0.58              |
| 58:s:39:LYS:HA    | 58:s:44:TYR:CD1   | 2.39                     | 0.58              |
| 65:z:82:GLY:CA    | 65:z:117:LEU:CD1  | 2.81                     | 0.58              |
| 2:1:7:HIS:HD2     | 2:1:10:ALA:HB2    | 1.68                     | 0.58              |
| 5:4:31:TYR:OH     | 43:d:103:U:O2'    | 2.20                     | 0.58              |
| 9:9:51:TYR:HB2    | 9:9:88:HIS:CB     | 2.32                     | 0.58              |
| 10:A:60:U:H4'     | 10:A:61:C:OP2     | 2.04                     | 0.58              |
| 17:D:439:U:O2     | 17:D:440:C:C5     | 2.56                     | 0.58              |
| 18:E:61:GLN:NE2   | 18:E:66:LEU:HD22  | 2.18                     | 0.58              |
| 29:P:22:THR:O     | 29:P:26:VAL:HG23  | 2.03                     | 0.58              |
| 38:Y:116:MET:HG2  | 38:Y:124:MET:CB   | 2.34                     | 0.58              |
| 60:u:55:MET:CE    | 60:u:60:ARG:HG2   | 2.33                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:5:9:DG:P         | 11:AA:470:ARG:HA   | 2.43                     | 0.58              |
| 8:7:10:U:H5''      | 8:7:10:U:O2        | 2.03                     | 0.58              |
| 28:O:49:ARG:HB3    | 28:O:53:GLU:OE2    | 2.02                     | 0.58              |
| 33:T:21:ASP:OD1    | 33:T:22:THR:N      | 2.34                     | 0.58              |
| 38:Y:102:ARG:CG    | 38:Y:141:ASP:HA    | 2.33                     | 0.58              |
| 55:p:149:ARG:NH2   | 55:p:162:VAL:N     | 2.52                     | 0.58              |
| 57:r:97:ARG:NH1    | 57:r:101:ASP:OD2   | 2.37                     | 0.58              |
| 58:s:132:HIS:O     | 58:s:135:GLN:HB2   | 2.03                     | 0.58              |
| 6:5:10:DT:O3'      | 12:AB:68:THR:CA    | 2.51                     | 0.58              |
| 8:7:7:U:H5''       | 8:7:7:U:C6         | 2.39                     | 0.58              |
| 9:9:24:SER:HB2     | 9:9:86:MET:HA      | 1.86                     | 0.58              |
| 12:AB:77:HIS:NE2   | 14:AE:297:ARG:NH2  | 2.51                     | 0.58              |
| 14:AE:506:VAL:HG23 | 14:AE:628:GLY:HA3  | 1.83                     | 0.58              |
| 17:D:588:G:H4'     | 27:N:3:MET:CE      | 2.33                     | 0.58              |
| 17:D:915:A:N6      | 17:D:916:U:C4      | 2.72                     | 0.58              |
| 17:D:972:C:O2'     | 29:P:57:VAL:HG13   | 2.03                     | 0.58              |
| 17:D:1107:C:P      | 22:I:172:ARG:HG3   | 2.43                     | 0.58              |
| 17:D:1308:U:P      | 37:X:98:ARG:HG3    | 2.43                     | 0.58              |
| 24:K:146:ASN:OD1   | 24:K:147:MET:N     | 2.37                     | 0.58              |
| 30:Q:87:LYS:HG3    | 30:Q:113:VAL:HG23  | 1.86                     | 0.58              |
| 35:V:4:LYS:HD2     | 35:V:5:ILE:HG23    | 1.85                     | 0.58              |
| 40:a:1028:A:H2'    | 40:a:1029:A:C8     | 2.37                     | 0.58              |
| 46:g:37:CYS:N      | 46:g:40:CYS:SG     | 2.71                     | 0.58              |
| 51:l:170:ARG:CZ    | 51:l:175:ILE:HA    | 2.33                     | 0.58              |
| 57:r:37:VAL:HG12   | 57:r:43:ASN:HD21   | 1.68                     | 0.58              |
| 58:s:120:ARG:CZ    | 58:s:120:ARG:HB2   | 2.34                     | 0.58              |
| 61:v:49:ALA:O      | 61:v:52:ALA:N      | 2.37                     | 0.58              |
| 2:1:11:ARG:NH1     | 2:1:98:LYS:HE3     | 2.19                     | 0.58              |
| 6:5:25:DA:C2       | 7:6:5:DG:C2        | 2.92                     | 0.58              |
| 9:9:73:LYS:CG      | 9:9:117:LEU:HD12   | 2.32                     | 0.58              |
| 11:AA:838:CYS:HB2  | 11:AA:918:LEU:HD22 | 1.85                     | 0.58              |
| 17:D:829:G:O3'     | 20:G:23:TRP:CZ2    | 2.56                     | 0.58              |
| 22:I:24:ALA:C      | 22:I:29:PHE:HE2    | 2.11                     | 0.58              |
| 26:M:24:ALA:O      | 26:M:27:VAL:HG22   | 2.04                     | 0.58              |
| 27:N:52:GLU:OE1    | 27:N:53:GLY:N      | 2.37                     | 0.58              |
| 33:T:32:LEU:HD11   | 33:T:62:GLN:OE1    | 2.04                     | 0.58              |
| 44:e:2:LYS:HD2     | 44:e:6:LEU:HD11    | 1.85                     | 0.58              |
| 45:f:10:THR:HG22   | 45:f:54:MET:C      | 2.27                     | 0.58              |
| 57:r:30:LEU:HD23   | 57:r:35:LYS:HE2    | 1.85                     | 0.58              |
| 58:s:53:TYR:CD1    | 58:s:121:LYS:HD2   | 2.39                     | 0.58              |
| 1:0:16:GLU:C       | 1:0:18:GLN:OE1     | 2.46                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:3:6:ARG:NH1      | 40:a:84:A:O2'      | 2.36                     | 0.58              |
| 4:3:94:ARG:HB3     | 4:3:103:ILE:HD12   | 1.86                     | 0.58              |
| 9:9:4:ASN:HB3      | 9:9:8:LYS:NZ       | 2.19                     | 0.58              |
| 21:H:75:VAL:HG23   | 21:H:81:GLU:OE2    | 2.04                     | 0.58              |
| 24:K:10:GLU:OE1    | 24:K:10:GLU:N      | 2.35                     | 0.58              |
| 27:N:7:ILE:HB      | 27:N:77:ARG:NH1    | 2.18                     | 0.58              |
| 27:N:8:ALA:O       | 27:N:12:THR:HG23   | 2.03                     | 0.58              |
| 28:O:94:LEU:O      | 28:O:98:LEU:HD13   | 2.04                     | 0.58              |
| 40:a:2189:U:O4'    | 40:a:2189:U:OP1    | 2.21                     | 0.58              |
| 40:a:2189:U:O2'    | 40:a:2190:G:O4'    | 2.22                     | 0.58              |
| 40:a:2395:C:H2'    | 40:a:2396:G:O4'    | 2.03                     | 0.58              |
| 40:a:2547:A:H2'    | 40:a:2548:U:C6     | 2.38                     | 0.58              |
| 44:e:18:LEU:HD11   | 44:e:54:LYS:HE3    | 1.86                     | 0.58              |
| 58:s:133:ALA:C     | 58:s:135:GLN:N     | 2.60                     | 0.58              |
| 59:t:121:GLU:OE2   | 64:y:41:GLN:NE2    | 2.37                     | 0.58              |
| 12:AB:6:LEU:H      | 12:AB:88:VAL:HG21  | 1.69                     | 0.58              |
| 17:D:1082:A:OP1    | 24:K:23:LYS:NZ     | 2.34                     | 0.58              |
| 20:G:35:ARG:HD2    | 21:H:14:LYS:CE     | 2.34                     | 0.58              |
| 40:a:607:U:C5      | 40:a:620:G:C4      | 2.91                     | 0.58              |
| 40:a:1021:A:N1     | 40:a:1141:U:O4     | 2.37                     | 0.58              |
| 60:u:91:ASP:O      | 60:u:95:LEU:HD23   | 2.03                     | 0.58              |
| 8:7:15:U:C2        | 15:AF:83:VAL:HG12  | 2.19                     | 0.58              |
| 9:9:23:LEU:N       | 9:9:118:ILE:HD11   | 2.19                     | 0.58              |
| 10:A:15:G:N1       | 10:A:20:U:O2       | 2.37                     | 0.58              |
| 12:AB:137:ALA:HA   | 12:AB:156:ASN:HA   | 1.86                     | 0.58              |
| 12:AB:141:LEU:O    | 12:AB:151:LYS:HA   | 2.04                     | 0.58              |
| 17:D:695:A:H8      | 17:D:695:A:H5''    | 1.68                     | 0.58              |
| 18:E:61:GLN:HE21   | 18:E:66:LEU:HD22   | 1.69                     | 0.58              |
| 24:K:156:LYS:HA    | 27:N:66:PHE:CD2    | 2.39                     | 0.58              |
| 30:Q:52:PHE:CD2    | 30:Q:56:ARG:HG2    | 2.39                     | 0.58              |
| 40:a:2259:U:N3     | 40:a:2260:C:C5     | 2.71                     | 0.58              |
| 49:j:46:ARG:NH1    | 49:j:85:ALA:O      | 2.32                     | 0.58              |
| 52:m:12:ARG:NE     | 52:m:44:VAL:HG21   | 2.19                     | 0.58              |
| 4:3:7:ARG:HH22     | 40:a:98:G:N2       | 2.00                     | 0.57              |
| 14:AE:1143:ASP:OD1 | 14:AE:1148:ARG:NH1 | 2.37                     | 0.57              |
| 16:C:13:PHE:HB3    | 16:C:51:TYR:CD1    | 2.39                     | 0.57              |
| 17:D:1145:A:O2'    | 17:D:1146:A:O5'    | 2.18                     | 0.57              |
| 24:K:136:VAL:O     | 24:K:140:THR:HG23  | 2.04                     | 0.57              |
| 38:Y:32:VAL:HG22   | 38:Y:60:VAL:CG2    | 2.34                     | 0.57              |
| 40:a:1565:C:OP1    | 47:h:18:LYS:NZ     | 2.26                     | 0.57              |
| 43:d:48:U:H2'      | 43:d:49:C:C6       | 2.39                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 45:f:40:ASP:OD1    | 45:f:45:ARG:NH2   | 2.37                     | 0.57              |
| 49:j:55:LYS:HZ1    | 49:j:59:ARG:C     | 2.11                     | 0.57              |
| 51:l:17:THR:HA     | 51:l:21:ARG:NH2   | 2.19                     | 0.57              |
| 60:u:61:LEU:HB3    | 60:u:62:PRO:HD2   | 1.85                     | 0.57              |
| 2:1:73:LYS:C       | 2:1:74:ILE:HD12   | 2.29                     | 0.57              |
| 11:AA:1254:VAL:O   | 14:AE:99:ARG:NH2  | 2.37                     | 0.57              |
| 17:D:974:A:OP1     | 32:S:69:ARG:NH1   | 2.37                     | 0.57              |
| 20:G:66:LYS:HB3    | 20:G:154:MET:CE   | 2.34                     | 0.57              |
| 20:G:107:VAL:O     | 20:G:111:ILE:HG12 | 2.04                     | 0.57              |
| 26:M:28:ASN:HA     | 26:M:31:MET:HE3   | 1.85                     | 0.57              |
| 31:R:110:ARG:NE    | 31:R:117:TYR:HD2  | 2.02                     | 0.57              |
| 32:S:90:ARG:C      | 32:S:92:GLU:OE1   | 2.47                     | 0.57              |
| 34:U:12:LYS:CD     | 34:U:13:LYS:HG2   | 2.33                     | 0.57              |
| 40:a:832:U:H2'     | 40:a:833:A:H8     | 1.69                     | 0.57              |
| 40:a:1065:U:O2'    | 40:a:1066:U:O5'   | 2.16                     | 0.57              |
| 40:a:1682:G:H2'    | 40:a:1683:U:C6    | 2.39                     | 0.57              |
| 40:a:2816:G:O4'    | 48:i:41:HIS:CE1   | 2.57                     | 0.57              |
| 51:l:148:ILE:HD13  | 51:l:187:VAL:HB   | 1.85                     | 0.57              |
| 61:v:97:GLN:H      | 61:v:100:LYS:HZ1  | 1.51                     | 0.57              |
| 7:6:23:DC:H5''     | 14:AE:259:ARG:NH1 | 1.92                     | 0.57              |
| 8:7:12:U:H3'       | 8:7:12:U:H6       | 1.69                     | 0.57              |
| 10:B:30:G:O2'      | 17:D:1339:A:C2    | 2.52                     | 0.57              |
| 16:C:16:GLU:OE1    | 16:C:18:VAL:N     | 2.36                     | 0.57              |
| 19:F:16:LEU:C      | 19:F:20:LYS:HZ3   | 2.12                     | 0.57              |
| 20:G:52:GLU:O      | 20:G:56:GLU:OE1   | 2.23                     | 0.57              |
| 26:M:66:LEU:HD11   | 26:M:100:ALA:HB3  | 1.85                     | 0.57              |
| 28:O:5:GLN:NE2     | 28:O:20:PHE:CB    | 2.67                     | 0.57              |
| 33:T:28:GLN:HB2    | 33:T:66:LEU:HD21  | 1.86                     | 0.57              |
| 40:a:500:G:N1      | 40:a:503:A:OP2    | 2.37                     | 0.57              |
| 40:a:1824:G:H5''   | 47:h:52:ARG:HH22  | 1.69                     | 0.57              |
| 40:a:2683:C:H4'    | 49:j:13:ARG:CZ    | 2.34                     | 0.57              |
| 41:b:55:ARG:NE     | 41:b:55:ARG:HA    | 2.19                     | 0.57              |
| 54:o:55:LEU:HD21   | 54:o:59:ILE:HD11  | 1.87                     | 0.57              |
| 61:v:26:VAL:HG13   | 61:v:104:GLU:CD   | 2.29                     | 0.57              |
| 11:AA:1223:ARG:NH2 | 14:AE:721:SER:OG  | 2.38                     | 0.57              |
| 22:I:82:GLU:O      | 22:I:86:LYS:HD3   | 2.04                     | 0.57              |
| 29:P:86:ALA:O      | 29:P:90:LEU:CD1   | 2.53                     | 0.57              |
| 34:U:14:ARG:HD3    | 34:U:42:ILE:HG21  | 1.86                     | 0.57              |
| 40:a:5:A:H2'       | 40:a:6:A:C8       | 2.39                     | 0.57              |
| 40:a:1141:U:H5     | 58:s:68:LYS:NZ    | 2.02                     | 0.57              |
| 40:a:1198:U:H2'    | 40:a:1199:U:C6    | 2.40                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:a:1278:C:O2'   | 62:w:27:SER:OG     | 2.16                     | 0.57              |
| 40:a:2349:G:C6    | 40:a:2369:A:C6     | 2.92                     | 0.57              |
| 62:w:9:GLN:O      | 62:w:17:ARG:HD3    | 2.05                     | 0.57              |
| 5:4:46:LYS:O      | 5:4:50:MET:HG2     | 2.04                     | 0.57              |
| 5:4:60:VAL:HG12   | 5:4:71:LYS:HE2     | 1.85                     | 0.57              |
| 11:AA:13:LYS:HB2  | 11:AA:1180:MET:HE2 | 1.86                     | 0.57              |
| 12:AB:89:PRO:HG2  | 14:AE:290:ILE:CG2  | 2.33                     | 0.57              |
| 17:D:562:U:C3'    | 31:R:14:ARG:HH11   | 2.18                     | 0.57              |
| 21:H:273:ARG:HD3  | 21:H:280:LEU:HD11  | 1.85                     | 0.57              |
| 21:H:280:LEU:N    | 21:H:330:VAL:O     | 2.31                     | 0.57              |
| 23:J:196:ASN:ND2  | 23:J:199:LEU:HG    | 2.20                     | 0.57              |
| 25:L:14:GLN:OE1   | 25:L:83:ALA:HA     | 2.04                     | 0.57              |
| 35:V:11:ARG:HE    | 35:V:58:VAL:HG22   | 1.69                     | 0.57              |
| 40:a:811:U:H2'    | 60:u:21:ARG:HA     | 1.86                     | 0.57              |
| 57:r:135:HIS:ND1  | 57:r:137:GLU:CD    | 2.44                     | 0.57              |
| 12:AB:148:LYS:NZ  | 29:P:102:LEU:O     | 2.36                     | 0.57              |
| 17:D:280:C:O2     | 35:V:40:ARG:NH2    | 2.37                     | 0.57              |
| 17:D:1356:G:H2'   | 17:D:1357:A:C8     | 2.40                     | 0.57              |
| 22:I:85:GLU:OE2   | 22:I:88:ARG:NH1    | 2.26                     | 0.57              |
| 26:M:23:LEU:HD12  | 26:M:23:LEU:H      | 1.70                     | 0.57              |
| 26:M:26:PHE:CD1   | 26:M:101:MET:SD    | 2.97                     | 0.57              |
| 38:Y:58:ILE:HG23  | 38:Y:66:PHE:CE2    | 2.40                     | 0.57              |
| 40:a:580:U:H2'    | 40:a:581:C:H6      | 1.69                     | 0.57              |
| 40:a:593:U:H2'    | 40:a:594:U:C6      | 2.39                     | 0.57              |
| 43:d:106:G:H2'    | 43:d:107:G:O4'     | 2.04                     | 0.57              |
| 61:v:105:MET:HE2  | 61:v:108:VAL:HG21  | 1.87                     | 0.57              |
| 3:2:56:GLU:CD     | 3:2:87:LEU:C       | 2.73                     | 0.57              |
| 5:4:48:MET:HE3    | 5:4:84:PRO:O       | 2.04                     | 0.57              |
| 9:9:38:MET:SD     | 38:Y:117:THR:HG22  | 2.45                     | 0.57              |
| 11:AA:1122:LYS:NZ | 11:AA:1126:ASP:OD1 | 2.38                     | 0.57              |
| 12:AB:102:LYS:CE  | 14:AE:285:LEU:HA   | 2.34                     | 0.57              |
| 12:AB:102:LYS:HE2 | 14:AE:285:LEU:CA   | 2.34                     | 0.57              |
| 16:C:60:LYS:HZ1   | 17:D:735:C:C4'     | 2.16                     | 0.57              |
| 29:P:63:ASP:OD2   | 29:P:64:GLN:N      | 2.38                     | 0.57              |
| 38:Y:45:THR:HG21  | 38:Y:50:LYS:HZ2    | 1.70                     | 0.57              |
| 40:a:2093:G:P     | 57:r:22:LYS:HZ2    | 2.20                     | 0.57              |
| 40:a:2514:U:H2'   | 40:a:2515:C:C6     | 2.40                     | 0.57              |
| 50:k:34:LEU:H     | 50:k:51:GLU:CD     | 2.12                     | 0.57              |
| 61:v:41:LEU:CD2   | 61:v:45:GLN:HE22   | 2.18                     | 0.57              |
| 61:v:49:ALA:C     | 61:v:53:MET:HE1    | 2.30                     | 0.57              |
| 65:z:53:ARG:CG    | 65:z:57:PHE:HE2    | 2.18                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:15:SER:HB2    | 1:0:18:GLN:NE2    | 2.19                     | 0.57              |
| 3:2:54:GLU:OE1    | 3:2:54:GLU:N      | 2.38                     | 0.57              |
| 9:9:122:GLN:HG2   | 9:9:123:ILE:H     | 1.70                     | 0.57              |
| 25:L:95:ALA:O     | 25:L:96:VAL:C     | 2.47                     | 0.57              |
| 38:Y:116:MET:HB3  | 38:Y:124:MET:HE2  | 1.87                     | 0.57              |
| 40:a:228:C:N4     | 40:a:2407:A:N3    | 2.52                     | 0.57              |
| 40:a:628:G:C6     | 40:a:636:G:C2     | 2.92                     | 0.57              |
| 40:a:782:A:C2     | 47:h:225:MET:HE2  | 2.39                     | 0.57              |
| 40:a:1360:G:N7    | 40:a:1361:G:C8    | 2.73                     | 0.57              |
| 40:a:1869:G:N2    | 40:a:1871:A:O2'   | 2.37                     | 0.57              |
| 47:h:52:ARG:HE    | 47:h:53:HIS:CE1   | 2.23                     | 0.57              |
| 49:j:180:VAL:O    | 49:j:180:VAL:HG13 | 2.05                     | 0.57              |
| 58:s:31:GLU:OE2   | 58:s:35:ARG:NH1   | 2.37                     | 0.57              |
| 61:v:1:MET:HE3    | 61:v:1:MET:CA     | 2.34                     | 0.57              |
| 3:2:1:MET:N       | 40:a:142:A:O2'    | 2.33                     | 0.57              |
| 5:4:2:PHE:HE2     | 5:4:55:GLU:HG2    | 1.69                     | 0.57              |
| 10:B:70:G:H2'     | 10:B:71:C:H5''    | 1.85                     | 0.57              |
| 27:N:66:PHE:CG    | 27:N:67:GLN:OE1   | 2.57                     | 0.57              |
| 35:V:42:THR:HG22  | 35:V:44:LEU:CD1   | 2.34                     | 0.57              |
| 36:W:40:ILE:HG21  | 36:W:66:MET:SD    | 2.45                     | 0.57              |
| 38:Y:78:LEU:HD12  | 38:Y:112:LYS:HZ1  | 1.69                     | 0.57              |
| 40:a:64:A:H2'     | 40:a:65:U:C6      | 2.40                     | 0.57              |
| 40:a:78:U:H5''    | 44:e:4:LYS:NZ     | 2.20                     | 0.57              |
| 40:a:1818:U:OP2   | 47:h:156:ARG:CZ   | 2.53                     | 0.57              |
| 61:v:70:ASP:C     | 61:v:92:TRP:HZ3   | 2.13                     | 0.57              |
| 10:B:60:U:H4'     | 10:B:61:C:OP2     | 2.04                     | 0.57              |
| 17:D:439:U:O2     | 17:D:440:C:C6     | 2.58                     | 0.57              |
| 22:I:151:VAL:HG12 | 22:I:200:VAL:CG2  | 2.35                     | 0.57              |
| 30:Q:15:GLN:OE1   | 30:Q:78:GLY:HA3   | 2.05                     | 0.57              |
| 40:a:1442:U:H2'   | 40:a:1443:U:C6    | 2.40                     | 0.57              |
| 40:a:1568:G:N7    | 47:h:28:LYS:NZ    | 2.52                     | 0.57              |
| 43:d:5:U:OP1      | 43:d:61:G:O2'     | 2.16                     | 0.57              |
| 59:t:20:MET:HB3   | 59:t:44:LYS:CE    | 2.35                     | 0.57              |
| 64:y:51:ARG:HD3   | 64:y:58:ALA:HB3   | 1.86                     | 0.57              |
| 65:z:74:ILE:HG12  | 65:z:79:PHE:HB2   | 1.86                     | 0.57              |
| 11:AA:516:ASP:OD1 | 11:AA:516:ASP:O   | 2.23                     | 0.56              |
| 17:D:512:U:OP1    | 23:J:44:ARG:NH1   | 2.38                     | 0.56              |
| 17:D:911:U:H2'    | 17:D:912:C:C6     | 2.40                     | 0.56              |
| 20:G:131:LYS:HG3  | 20:G:132:LYS:HD2  | 1.87                     | 0.56              |
| 22:I:25:ASN:N     | 22:I:29:PHE:HE2   | 2.01                     | 0.56              |
| 40:a:2192:U:H2'   | 40:a:2193:G:C8    | 2.40                     | 0.56              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:9:124:ASP:OD2    | 9:9:126:LEU:HD21    | 2.05                     | 0.56              |
| 13:AC:82:LEU:HD11  | 13:AC:171:LEU:HD23  | 1.86                     | 0.56              |
| 10:B:5:G:H2'       | 10:B:6:G:C5'        | 2.36                     | 0.56              |
| 10:B:75:C:O2'      | 10:B:76:A:C8        | 2.58                     | 0.56              |
| 21:H:51:GLU:OE1    | 21:H:51:GLU:N       | 2.37                     | 0.56              |
| 32:S:63:ARG:NH2    | 32:S:68:GLY:O       | 2.32                     | 0.56              |
| 40:a:839:U:C2      | 40:a:840:C:C5       | 2.93                     | 0.56              |
| 40:a:839:U:H2'     | 40:a:840:C:C6       | 2.40                     | 0.56              |
| 40:a:2483:C:O2     | 61:v:51:ARG:NH2     | 2.38                     | 0.56              |
| 49:j:3:GLY:N       | 49:j:204:LYS:HE2    | 2.20                     | 0.56              |
| 52:m:24:THR:HG23   | 52:m:27:GLY:H       | 1.68                     | 0.56              |
| 57:r:6:LEU:HD11    | 57:r:37:VAL:CG2     | 2.33                     | 0.56              |
| 8:7:6:U:C2         | 17:D:1493:A:H2      | 2.24                     | 0.56              |
| 10:A:75:C:O2'      | 10:A:76:A:C8        | 2.58                     | 0.56              |
| 16:C:55:LEU:O      | 16:C:59:ILE:HG12    | 2.04                     | 0.56              |
| 17:D:193:C:O2'     | 18:E:59:ASP:OD2     | 2.23                     | 0.56              |
| 17:D:1145:A:HO2'   | 17:D:1146:A:P       | 2.27                     | 0.56              |
| 21:H:117:LYS:CB    | 21:H:279:LYS:O      | 2.54                     | 0.56              |
| 21:H:297:GLU:HG2   | 21:H:300:VAL:HG21   | 1.86                     | 0.56              |
| 22:I:6:HIS:HB3     | 32:S:89:MET:SD      | 2.45                     | 0.56              |
| 23:J:62:ARG:HA     | 23:J:72:PHE:CE1     | 2.41                     | 0.56              |
| 26:M:66:LEU:HD23   | 26:M:70:ARG:HH21    | 1.69                     | 0.56              |
| 29:P:21:ALA:O      | 29:P:24:GLU:HG3     | 2.04                     | 0.56              |
| 33:T:32:LEU:CD1    | 33:T:62:GLN:OE1     | 2.53                     | 0.56              |
| 33:T:35:GLN:CB     | 33:T:59:MET:HE1     | 2.35                     | 0.56              |
| 36:W:64:ASP:OD2    | 46:g:57:VAL:HG23    | 2.06                     | 0.56              |
| 37:X:28:THR:HG22   | 37:X:29:ARG:NH1     | 2.20                     | 0.56              |
| 40:a:3:U:H2'       | 40:a:4:U:H6         | 1.69                     | 0.56              |
| 40:a:16:C:C4'      | 48:i:15:MET:HE3     | 2.35                     | 0.56              |
| 40:a:659:G:H1'     | 51:l:100:MET:HE1    | 1.87                     | 0.56              |
| 40:a:1365:A:O2'    | 42:c:11:ARG:NH1     | 2.39                     | 0.56              |
| 41:b:51:VAL:C      | 41:b:62:LYS:NZ      | 2.63                     | 0.56              |
| 43:d:45:A:H5'      | 53:n:92:ARG:NH1     | 2.20                     | 0.56              |
| 49:j:91:THR:HB     | 49:j:94:GLN:HG2     | 1.87                     | 0.56              |
| 51:l:136:GLN:NE2   | 51:l:140:ASP:OD2    | 2.37                     | 0.56              |
| 58:s:74:TYR:CD2    | 58:s:74:TYR:N       | 2.69                     | 0.56              |
| 59:t:112:PHE:CD2   | 59:t:115:ILE:HD12   | 2.39                     | 0.56              |
| 61:v:37:GLY:C      | 61:v:126:ILE:HD11   | 2.30                     | 0.56              |
| 9:9:43:LYS:HD3     | 9:9:98:GLU:CG       | 2.35                     | 0.56              |
| 11:AA:839:VAL:HG12 | 11:AA:1049:ILE:HG12 | 1.87                     | 0.56              |
| 10:B:30:G:O2'      | 17:D:1339:A:H2      | 1.80                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:D:521:G:O5'    | 31:R:70:GLU:OE1   | 2.23                     | 0.56              |
| 23:J:121:LYS:HG2  | 23:J:131:ASN:ND2  | 2.20                     | 0.56              |
| 24:K:159:LYS:HZ3  | 27:N:44:GLY:HA3   | 1.71                     | 0.56              |
| 26:M:134:ALA:O    | 26:M:137:LYS:HG2  | 2.06                     | 0.56              |
| 29:P:15:HIS:HA    | 29:P:18:ILE:HG22  | 1.88                     | 0.56              |
| 40:a:1799:G:C2    | 47:h:154:LEU:HD23 | 2.41                     | 0.56              |
| 40:a:2071:A:H2'   | 40:a:2072:C:C6    | 2.40                     | 0.56              |
| 41:b:45:PHE:CD2   | 41:b:80:ILE:HD11  | 2.40                     | 0.56              |
| 53:n:163:ASP:OD1  | 53:n:164:GLU:N    | 2.39                     | 0.56              |
| 55:p:109:PHE:CE1  | 55:p:152:ARG:NH1  | 2.74                     | 0.56              |
| 62:w:67:PHE:O     | 62:w:71:ARG:N     | 2.39                     | 0.56              |
| 9:9:56:ARG:NH2    | 40:a:1084:A:C1'   | 2.69                     | 0.56              |
| 20:G:19:GLN:CG    | 21:H:76:GLU:HB3   | 2.34                     | 0.56              |
| 23:J:138:SER:O    | 23:J:141:ASP:OD1  | 2.24                     | 0.56              |
| 25:L:42:TRP:CZ2   | 25:L:102:MET:CG   | 2.88                     | 0.56              |
| 28:O:118:LEU:CD2  | 28:O:124:ARG:HA   | 2.35                     | 0.56              |
| 40:a:17:G:H2'     | 40:a:18:U:C6      | 2.41                     | 0.56              |
| 40:a:589:U:H2'    | 40:a:590:A:H8     | 1.71                     | 0.56              |
| 40:a:2720:U:OP1   | 64:y:53:ARG:NH2   | 2.38                     | 0.56              |
| 46:g:18:CYS:HB3   | 46:g:40:CYS:HB2   | 1.85                     | 0.56              |
| 55:p:85:LYS:HE3   | 55:p:164:TYR:CE1  | 2.41                     | 0.56              |
| 62:w:35:LYS:NZ    | 62:w:112:TYR:HE2  | 2.04                     | 0.56              |
| 5:4:55:GLU:O      | 5:4:59:GLU:OE1    | 2.24                     | 0.56              |
| 10:A:5:G:H2'      | 10:A:6:G:C5'      | 2.35                     | 0.56              |
| 17:D:440:C:C4     | 17:D:441:A:N7     | 2.73                     | 0.56              |
| 17:D:1366:C:O2'   | 29:P:62:ARG:NH2   | 2.37                     | 0.56              |
| 17:D:1515:G:H2'   | 17:D:1516:G:H8    | 1.70                     | 0.56              |
| 26:M:68:ASN:ND2   | 26:M:130:ASN:OD1  | 2.38                     | 0.56              |
| 33:T:10:LYS:O     | 33:T:14:GLU:OE1   | 2.23                     | 0.56              |
| 46:g:47:LYS:HG2   | 53:n:115:ARG:NH2  | 2.20                     | 0.56              |
| 50:k:8:LYS:HZ1    | 50:k:54:ILE:HG12  | 1.69                     | 0.56              |
| 51:l:42:GLY:CA    | 51:l:92:HIS:HE1   | 2.18                     | 0.56              |
| 54:o:30:ARG:HH12  | 60:u:62:PRO:HB3   | 1.70                     | 0.56              |
| 58:s:37:ARG:HD3   | 58:s:39:LYS:HD2   | 1.88                     | 0.56              |
| 59:t:12:ASP:CG    | 59:t:85:VAL:HG13  | 2.31                     | 0.56              |
| 5:4:77:VAL:HG11   | 5:4:79:ARG:NH2    | 2.21                     | 0.56              |
| 9:9:47:GLU:O      | 9:9:51:TYR:CE1    | 2.59                     | 0.56              |
| 12:AB:138:ARG:HD2 | 12:AB:154:VAL:O   | 2.05                     | 0.56              |
| 17:D:502:A:O3'    | 31:R:116:LYS:HE2  | 2.06                     | 0.56              |
| 17:D:588:G:C5'    | 27:N:3:MET:HE1    | 2.36                     | 0.56              |
| 18:E:61:GLN:HE21  | 18:E:66:LEU:CD2   | 2.18                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:H:163:ARG:CB   | 21:H:298:GLU:HG3  | 2.35                     | 0.56              |
| 24:K:148:ASN:ND2  | 24:K:153:VAL:HG12 | 2.20                     | 0.56              |
| 33:T:3:LEU:HB2    | 33:T:35:GLN:CD    | 2.31                     | 0.56              |
| 34:U:39:PHE:HD1   | 34:U:50:THR:HG22  | 1.70                     | 0.56              |
| 40:a:5:A:H2'      | 40:a:6:A:H8       | 1.70                     | 0.56              |
| 40:a:1570:A:H2'   | 40:a:1571:A:C8    | 2.40                     | 0.56              |
| 40:a:2849:U:P     | 64:y:93:ARG:NH2   | 2.78                     | 0.56              |
| 41:b:51:VAL:C     | 41:b:62:LYS:HZ3   | 2.13                     | 0.56              |
| 47:h:183:LYS:HE2  | 47:h:266:PHE:HA   | 1.88                     | 0.56              |
| 60:u:125:LEU:HD23 | 60:u:125:LEU:N    | 2.21                     | 0.56              |
| 12:AB:130:PHE:CD2 | 12:AB:152:HIS:HE1 | 2.23                     | 0.56              |
| 17:D:827:U:O4     | 17:D:872:A:N1     | 2.39                     | 0.56              |
| 17:D:1381:U:C2    | 17:D:1382:C:C6    | 2.94                     | 0.56              |
| 19:F:26:ALA:HB3   | 19:F:28:VAL:HG23  | 1.88                     | 0.56              |
| 21:H:116:VAL:HA   | 21:H:279:LYS:HD2  | 1.88                     | 0.56              |
| 30:Q:87:LYS:HG3   | 30:Q:113:VAL:CG2  | 2.35                     | 0.56              |
| 31:R:4:VAL:HG13   | 31:R:5:ASN:N      | 2.20                     | 0.56              |
| 40:a:84:A:N1      | 40:a:98:G:O2'     | 2.37                     | 0.56              |
| 40:a:784:G:H5'    | 40:a:785:G:OP1    | 2.06                     | 0.56              |
| 40:a:2291:U:H2'   | 40:a:2292:U:C6    | 2.40                     | 0.56              |
| 42:c:66:THR:O     | 42:c:70:GLU:OE1   | 2.23                     | 0.56              |
| 47:h:175:ARG:CG   | 47:h:181:MET:HE1  | 2.34                     | 0.56              |
| 48:i:40:ARG:HG3   | 48:i:41:HIS:ND1   | 2.21                     | 0.56              |
| 50:k:19:HIS:ND1   | 50:k:41:PRO:HD2   | 2.21                     | 0.56              |
| 55:p:94:TYR:CE1   | 55:p:107:LEU:O    | 2.59                     | 0.56              |
| 58:s:73:VAL:HG12  | 58:s:74:TYR:N     | 2.20                     | 0.56              |
| 64:y:106:LYS:HA   | 64:y:109:ARG:NH2  | 2.20                     | 0.56              |
| 4:3:6:ARG:CZ      | 40:a:84:A:H2'     | 2.35                     | 0.56              |
| 5:4:80:HIS:CE1    | 5:4:83:LYS:HG3    | 2.41                     | 0.56              |
| 8:7:18:U:O2       | 8:7:18:U:H2'      | 2.06                     | 0.56              |
| 14:AE:144:TYR:OH  | 14:AE:293:ARG:NH2 | 2.36                     | 0.56              |
| 20:G:19:GLN:HG3   | 21:H:76:GLU:CB    | 2.35                     | 0.56              |
| 20:G:35:ARG:HG2   | 20:G:40:ILE:HG13  | 1.87                     | 0.56              |
| 22:I:66:VAL:HB    | 22:I:101:ILE:HD12 | 1.88                     | 0.56              |
| 22:I:150:LYS:HE3  | 22:I:201:TRP:CZ3  | 2.41                     | 0.56              |
| 22:I:156:ARG:NH1  | 22:I:193:TYR:O    | 2.39                     | 0.56              |
| 24:K:74:VAL:HG11  | 24:K:144:LEU:HD12 | 1.88                     | 0.56              |
| 26:M:95:ARG:O     | 26:M:99:LEU:HG    | 2.05                     | 0.56              |
| 37:X:16:VAL:CG2   | 37:X:17:ILE:HD12  | 2.35                     | 0.56              |
| 39:Z:2:ILE:HB     | 39:Z:5:ASP:HB3    | 1.88                     | 0.56              |
| 40:a:1047:G:HO2'  | 40:a:1110:G:H1    | 1.54                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:a:1693:U:O2'   | 47:h:14:ARG:NH2   | 2.38                     | 0.56              |
| 41:b:21:LEU:HD21  | 41:b:41:ARG:NE    | 2.20                     | 0.56              |
| 44:e:2:LYS:HE2    | 44:e:52:ARG:HE    | 1.71                     | 0.56              |
| 44:e:23:ARG:HG3   | 44:e:24:GLU:N     | 2.21                     | 0.56              |
| 53:n:62:GLY:C     | 53:n:95:ARG:NH2   | 2.63                     | 0.56              |
| 58:s:73:VAL:C     | 58:s:74:TYR:HD2   | 2.14                     | 0.56              |
| 63:x:36:TYR:CD2   | 63:x:52:SER:HB2   | 2.41                     | 0.56              |
| 5:4:53:LYS:HB2    | 5:4:56:PHE:CE2    | 2.40                     | 0.56              |
| 9:9:27:VAL:HG13   | 9:9:27:VAL:O      | 2.05                     | 0.56              |
| 10:A:22:G:H2'     | 10:A:23:C:H6      | 1.70                     | 0.56              |
| 12:AB:26:VAL:HA   | 12:AB:58:GLU:OE1  | 2.05                     | 0.56              |
| 17:D:280:C:H1'    | 35:V:40:ARG:NH1   | 2.21                     | 0.56              |
| 17:D:946:A:H2'    | 17:D:947:G:C8     | 2.41                     | 0.56              |
| 35:V:64:CYS:HG    | 35:V:74:THR:HG1   | 1.51                     | 0.56              |
| 37:X:71:ARG:NE    | 46:g:50:ASP:O     | 2.39                     | 0.56              |
| 40:a:1038:G:H2'   | 40:a:1039:A:C8    | 2.42                     | 0.56              |
| 62:w:35:LYS:HZ2   | 62:w:112:TYR:HE2  | 1.52                     | 0.56              |
| 4:3:47:LYS:HE3    | 40:a:483:A:OP1    | 2.06                     | 0.55              |
| 4:3:69:ASN:ND2    | 40:a:329:G:OP2    | 2.37                     | 0.55              |
| 8:7:8:U:H5'       | 17:D:1397:C:C2    | 2.41                     | 0.55              |
| 10:B:18:G:H1'     | 10:B:58:A:C2      | 2.41                     | 0.55              |
| 17:D:1329:A:OP1   | 37:X:28:THR:HB    | 2.06                     | 0.55              |
| 21:H:116:VAL:CA   | 21:H:279:LYS:HD2  | 2.35                     | 0.55              |
| 22:I:31:ASP:HA    | 32:S:65:ARG:HH22  | 1.72                     | 0.55              |
| 22:I:140:ASN:O    | 22:I:144:LEU:HD23 | 2.06                     | 0.55              |
| 37:X:95:LEU:O     | 37:X:109:ARG:NH2  | 2.39                     | 0.55              |
| 40:a:2189:U:O2'   | 40:a:2190:G:C5'   | 2.54                     | 0.55              |
| 51:l:62:GLN:HA    | 51:l:69:ARG:NH2   | 2.20                     | 0.55              |
| 57:r:54:LEU:HA    | 57:r:57:LYS:NZ    | 2.20                     | 0.55              |
| 62:w:24:MET:HE2   | 62:w:34:ILE:HD13  | 1.87                     | 0.55              |
| 5:4:80:HIS:CD2    | 5:4:81:PRO:HD2    | 2.41                     | 0.55              |
| 6:5:15:DT:C2      | 11:AA:183:TRP:CD1 | 2.94                     | 0.55              |
| 8:7:1:A:H2'       | 8:7:2:U:H6        | 1.70                     | 0.55              |
| 11:AA:985:GLU:HB3 | 11:AA:988:LYS:HB2 | 1.88                     | 0.55              |
| 17:D:375:U:OP1    | 34:U:70:ARG:CG    | 2.54                     | 0.55              |
| 27:N:7:ILE:O      | 27:N:10:MET:HB3   | 2.05                     | 0.55              |
| 40:a:1857:G:O2'   | 40:a:1884:G:N2    | 2.38                     | 0.55              |
| 40:a:1980:G:O2'   | 40:a:1982:U:OP2   | 2.23                     | 0.55              |
| 40:a:2299:U:H2'   | 40:a:2300:C:H6    | 1.71                     | 0.55              |
| 43:d:42:C:C5'     | 53:n:64:LYS:HZ1   | 2.18                     | 0.55              |
| 5:4:57:TYR:CD2    | 61:v:136:MET:HE2  | 2.40                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:7:11:U:O2        | 8:7:11:U:H2'        | 2.06                     | 0.55              |
| 10:A:56:C:H1'      | 40:a:2112:G:C6      | 2.42                     | 0.55              |
| 17:D:110:C:O2'     | 34:U:25:ARG:O       | 2.21                     | 0.55              |
| 17:D:1071:C:H2'    | 17:D:1072:G:H8      | 1.71                     | 0.55              |
| 20:G:187:VAL:HG21  | 20:G:199:VAL:HG23   | 1.89                     | 0.55              |
| 21:H:100:LYS:O     | 21:H:104:ASP:N      | 2.38                     | 0.55              |
| 40:a:608:A:H2'     | 40:a:609:A:C8       | 2.41                     | 0.55              |
| 40:a:2315:G:H4'    | 53:n:127:ASN:HD22   | 1.71                     | 0.55              |
| 44:e:53:VAL:O      | 44:e:57:LEU:HD23    | 2.06                     | 0.55              |
| 3:2:56:GLU:CD      | 3:2:88:LYS:HA       | 2.31                     | 0.55              |
| 4:3:26:LYS:HE2     | 4:3:26:LYS:HA       | 1.88                     | 0.55              |
| 5:4:80:HIS:ND1     | 5:4:83:LYS:N        | 2.55                     | 0.55              |
| 9:9:98:GLU:HA      | 9:9:101:LYS:NZ      | 2.22                     | 0.55              |
| 9:9:112:ALA:O      | 9:9:123:ILE:CD1     | 2.54                     | 0.55              |
| 11:AA:1070:HIS:NE2 | 11:AA:1114:GLU:OE1  | 2.36                     | 0.55              |
| 17:D:321:A:N7      | 17:D:328:C:O2'      | 2.38                     | 0.55              |
| 21:H:268:VAL:HG23  | 21:H:269:ALA:H      | 1.72                     | 0.55              |
| 27:N:7:ILE:O       | 27:N:11:LEU:HD13    | 2.06                     | 0.55              |
| 30:Q:61:PHE:O      | 30:Q:64:GLN:HG2     | 2.06                     | 0.55              |
| 40:a:930:G:H1'     | 45:f:25:LEU:HD21    | 1.87                     | 0.55              |
| 40:a:1289:C:C2     | 40:a:1290:C:C5      | 2.94                     | 0.55              |
| 40:a:2517:C:C2     | 40:a:2542:A:N6      | 2.74                     | 0.55              |
| 40:a:2803:G:H2'    | 40:a:2804:U:C6      | 2.41                     | 0.55              |
| 45:f:7:ILE:CG2     | 45:f:55:VAL:HG21    | 2.35                     | 0.55              |
| 49:j:11:MET:SD     | 49:j:11:MET:C       | 2.90                     | 0.55              |
| 54:o:16:LYS:HD2    | 54:o:65:ALA:HB1     | 1.88                     | 0.55              |
| 61:v:96:ILE:HA     | 61:v:100:LYS:NZ     | 2.21                     | 0.55              |
| 63:x:21:LEU:HD22   | 63:x:23:ALA:HB2     | 1.87                     | 0.55              |
| 6:5:10:DT:O3'      | 12:AB:68:THR:C      | 2.47                     | 0.55              |
| 10:A:22:G:O2'      | 10:A:23:C:P         | 2.65                     | 0.55              |
| 11:AA:818:VAL:HG22 | 11:AA:1096:ILE:HG12 | 1.87                     | 0.55              |
| 17:D:276:G:H5'     | 35:V:17:MET:CE      | 2.36                     | 0.55              |
| 17:D:692:U:N3      | 17:D:695:A:OP2      | 2.34                     | 0.55              |
| 17:D:1076:U:OP1    | 20:G:174:LYS:NZ     | 2.40                     | 0.55              |
| 18:E:6:SER:O       | 18:E:10:ARG:HG2     | 2.07                     | 0.55              |
| 19:F:19:PHE:CE2    | 30:Q:110:ILE:HG22   | 2.42                     | 0.55              |
| 21:H:268:VAL:HG23  | 21:H:269:ALA:N      | 2.22                     | 0.55              |
| 32:S:27:LEU:HD21   | 32:S:48:LEU:N       | 2.21                     | 0.55              |
| 40:a:851:C:H2'     | 40:a:852:U:H6       | 1.72                     | 0.55              |
| 40:a:960:A:H61     | 61:v:82:MET:HE1     | 1.71                     | 0.55              |
| 40:a:2335:A:OP2    | 63:x:13:ARG:HB3     | 2.06                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:a:2591:C:H2'    | 40:a:2592:G:C8     | 2.42                     | 0.55              |
| 40:a:2742:G:P      | 56:q:36:ARG:NH1    | 2.80                     | 0.55              |
| 54:o:30:ARG:NH1    | 60:u:62:PRO:HB3    | 2.21                     | 0.55              |
| 59:t:59:LYS:HD2    | 59:t:89:ASN:HA     | 1.87                     | 0.55              |
| 3:2:2:ILE:HG21     | 3:2:42:GLU:OE1     | 2.06                     | 0.55              |
| 5:4:57:TYR:CB      | 61:v:136:MET:CE    | 2.84                     | 0.55              |
| 6:5:10:DT:O3'      | 12:AB:68:THR:HA    | 2.03                     | 0.55              |
| 12:AB:112:PRO:HB3  | 12:AB:132:GLU:OE1  | 2.07                     | 0.55              |
| 12:AB:116:VAL:HG23 | 12:AB:130:PHE:CE2  | 2.41                     | 0.55              |
| 13:AC:28:LEU:HD22  | 13:AC:201:LEU:HD23 | 1.88                     | 0.55              |
| 10:B:22:G:H2'      | 10:B:23:C:H6       | 1.70                     | 0.55              |
| 17:D:671:G:O3'     | 25:L:79:ARG:NH2    | 2.39                     | 0.55              |
| 17:D:713:G:H2'     | 17:D:714:G:C8      | 2.42                     | 0.55              |
| 26:M:71:PRO:HG3    | 26:M:103:TRP:CH2   | 2.42                     | 0.55              |
| 29:P:26:VAL:O      | 29:P:30:LYS:HG3    | 2.07                     | 0.55              |
| 29:P:47:GLU:OE1    | 29:P:67:ILE:O      | 2.24                     | 0.55              |
| 33:T:80:GLN:O      | 33:T:84:ARG:HG2    | 2.05                     | 0.55              |
| 40:a:64:A:H2'      | 40:a:65:U:H6       | 1.71                     | 0.55              |
| 40:a:1321:A:C4     | 40:a:1322:A:C8     | 2.94                     | 0.55              |
| 40:a:1349:C:C2     | 40:a:1350:C:C5     | 2.95                     | 0.55              |
| 40:a:1708:C:C2     | 40:a:1709:U:C5     | 2.95                     | 0.55              |
| 40:a:2557:G:H2'    | 40:a:2558:C:C6     | 2.42                     | 0.55              |
| 44:e:2:LYS:HE2     | 44:e:49:ASP:HA     | 1.88                     | 0.55              |
| 47:h:67:PHE:CE1    | 47:h:105:LEU:HD11  | 2.42                     | 0.55              |
| 49:j:78:GLY:C      | 49:j:79:LEU:HD22   | 2.32                     | 0.55              |
| 51:l:1:MET:HE1     | 51:l:20:GLY:N      | 2.21                     | 0.55              |
| 57:r:4:ILE:HD12    | 57:r:17:ASP:O      | 2.05                     | 0.55              |
| 58:s:13:ARG:CZ     | 58:s:49:ASP:O      | 2.54                     | 0.55              |
| 64:y:9:GLU:OE2     | 64:y:55:LEU:N      | 2.37                     | 0.55              |
| 4:3:48:PRO:HG3     | 4:3:56:GLY:HA3     | 1.89                     | 0.55              |
| 9:9:24:SER:CB      | 9:9:86:MET:HE2     | 2.36                     | 0.55              |
| 10:A:16:C:O2       | 40:a:2181:U:H5'    | 2.06                     | 0.55              |
| 10:A:37:A:H2'      | 10:A:38:A:O4'      | 2.07                     | 0.55              |
| 12:AB:4:TRP:CD2    | 12:AB:27:ASN:ND2   | 2.75                     | 0.55              |
| 16:C:39:ILE:HD12   | 17:D:719:C:O2      | 2.07                     | 0.55              |
| 17:D:672:U:O2'     | 17:D:673:A:H5'     | 2.06                     | 0.55              |
| 17:D:750:C:N3      | 17:D:751:U:C5      | 2.75                     | 0.55              |
| 20:G:27:MET:CE     | 20:G:187:VAL:HG12  | 2.37                     | 0.55              |
| 20:G:30:PHE:CD1    | 20:G:45:LYS:NZ     | 2.74                     | 0.55              |
| 27:N:7:ILE:O       | 27:N:11:LEU:CD1    | 2.55                     | 0.55              |
| 38:Y:15:GLY:HA2    | 38:Y:50:LYS:CG     | 2.33                     | 0.55              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 40:a:857:G:H5''  | 41:b:78:LYS:HZ2    | 1.72                     | 0.55              |
| 40:a:923:G:O4'   | 41:b:29:GLU:OE2    | 2.24                     | 0.55              |
| 40:a:1059:G:H2'  | 40:a:1060:U:C5     | 2.41                     | 0.55              |
| 40:a:1665:A:O3'  | 59:t:66:LYS:HD3    | 2.07                     | 0.55              |
| 46:g:2:LYS:HB2   | 46:g:5:ILE:HD11    | 1.88                     | 0.55              |
| 56:q:1:MET:HE1   | 56:q:35:GLN:C      | 2.32                     | 0.55              |
| 64:y:15:GLN:NE2  | 64:y:16:ASP:OD1    | 2.40                     | 0.55              |
| 2:l:43:ALA:O     | 2:l:47:VAL:HG12    | 2.07                     | 0.55              |
| 12:AB:8:TYR:OH   | 14:AE:278:ARG:NH2  | 2.40                     | 0.55              |
| 14:AE:287:ALA:CB | 14:AE:292:VAL:HG22 | 2.37                     | 0.55              |
| 17:D:1370:G:C2   | 17:D:1371:G:C8     | 2.95                     | 0.55              |
| 20:G:5:SER:OG    | 20:G:8:ASP:OD2     | 2.24                     | 0.55              |
| 24:K:99:ALA:HB2  | 24:K:124:LEU:HG    | 1.88                     | 0.55              |
| 37:X:28:THR:O    | 37:X:31:LYS:HG2    | 2.07                     | 0.55              |
| 37:X:95:LEU:HB3  | 37:X:96:PRO:CD     | 2.37                     | 0.55              |
| 40:a:1433:A:H2'  | 40:a:1434:A:O4'    | 2.07                     | 0.55              |
| 40:a:1567:G:OP2  | 47:h:83:TYR:OH     | 2.18                     | 0.55              |
| 40:a:1720:U:H2'  | 40:a:1721:G:O4'    | 2.06                     | 0.55              |
| 40:a:1774:C:O2   | 40:a:1774:C:H2'    | 2.07                     | 0.55              |
| 44:e:56:LEU:O    | 44:e:59:GLU:HG3    | 2.06                     | 0.55              |
| 47:h:157:SER:O   | 47:h:195:VAL:HG11  | 2.07                     | 0.55              |
| 49:j:156:PHE:CD2 | 58:s:81:ILE:HD13   | 2.42                     | 0.55              |
| 59:t:35:VAL:HG23 | 59:t:63:VAL:HA     | 1.89                     | 0.55              |
| 59:t:59:LYS:CD   | 59:t:89:ASN:HA     | 2.36                     | 0.55              |
| 10:A:60:U:P      | 10:A:61:C:H41      | 2.30                     | 0.55              |
| 10:A:76:A:N1     | 40:a:2422:C:C6     | 2.75                     | 0.55              |
| 12:AB:54:TYR:HE2 | 14:AE:291:ILE:CG2  | 2.13                     | 0.55              |
| 12:AB:78:PHE:CD1 | 12:AB:85:PRO:HB3   | 2.42                     | 0.55              |
| 12:AB:123:PHE:CZ | 29:P:85:ASP:CB     | 2.79                     | 0.55              |
| 10:B:75:C:P      | 40:a:2602:A:O2'    | 2.61                     | 0.55              |
| 17:D:50:A:O2'    | 17:D:360:G:N2      | 2.40                     | 0.55              |
| 17:D:324:G:N1    | 17:D:327:A:OP2     | 2.39                     | 0.55              |
| 17:D:1078:U:O3'  | 24:K:138:ARG:NH2   | 2.40                     | 0.55              |
| 19:F:19:PHE:CE1  | 19:F:23:CYS:SG     | 3.00                     | 0.55              |
| 21:H:5:PHE:O     | 21:H:9:PHE:HD1     | 1.90                     | 0.55              |
| 30:Q:46:THR:OG1  | 30:Q:49:GLY:N      | 2.34                     | 0.55              |
| 32:S:87:ALA:HB1  | 32:S:93:ILE:HG13   | 1.87                     | 0.55              |
| 40:a:150:U:H2'   | 40:a:151:C:H6      | 1.72                     | 0.55              |
| 40:a:888:C:N4    | 40:a:889:C:N4      | 2.55                     | 0.55              |
| 40:a:2683:C:H4'  | 49:j:13:ARG:NH2    | 2.22                     | 0.55              |
| 44:e:20:ASN:O    | 44:e:23:ARG:HG2    | 2.06                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:g:5:ILE:CD1     | 53:n:64:LYS:HE3    | 2.36                     | 0.55              |
| 49:j:55:LYS:NZ     | 49:j:60:VAL:N      | 2.55                     | 0.55              |
| 1:0:10:LYS:HE2     | 40:a:996:A:OP1     | 2.07                     | 0.55              |
| 8:7:6:U:C2         | 17:D:1493:A:C2     | 2.95                     | 0.55              |
| 10:B:37:A:H2'      | 10:B:38:A:O4'      | 2.07                     | 0.55              |
| 18:E:32:ILE:HG23   | 18:E:75:HIS:NE2    | 2.21                     | 0.55              |
| 18:E:78:ASN:C      | 18:E:82:GLN:OE1    | 2.50                     | 0.55              |
| 21:H:9:PHE:O       | 21:H:13:LEU:HD23   | 2.07                     | 0.55              |
| 24:K:45:ARG:C      | 24:K:71:MET:HE2    | 2.31                     | 0.55              |
| 25:L:99:ALA:HB3    | 25:L:104:LYS:NZ    | 2.22                     | 0.55              |
| 31:R:27:CYS:SG     | 31:R:30:LYS:NZ     | 2.68                     | 0.55              |
| 34:U:23:ASP:HB3    | 34:U:26:ASN:OD1    | 2.07                     | 0.55              |
| 37:X:93:ARG:CG     | 37:X:95:LEU:HD23   | 2.35                     | 0.55              |
| 38:Y:123:ALA:O     | 38:Y:126:ARG:HG3   | 2.07                     | 0.55              |
| 40:a:589:U:H2'     | 40:a:590:A:C8      | 2.42                     | 0.55              |
| 40:a:1348:C:C5     | 40:a:1349:C:C5     | 2.95                     | 0.55              |
| 41:b:68:LYS:HZ2    | 41:b:70:GLU:CD     | 2.13                     | 0.55              |
| 47:h:62:TYR:CD2    | 47:h:64:ILE:HD13   | 2.41                     | 0.55              |
| 51:l:147:LEU:HD11  | 51:l:170:ARG:HD2   | 1.89                     | 0.55              |
| 8:7:1:A:C4         | 8:7:2:U:C5         | 2.95                     | 0.54              |
| 9:9:23:LEU:HD21    | 9:9:96:PHE:CD1     | 2.42                     | 0.54              |
| 11:AA:103:VAL:HB   | 11:AA:114:VAL:HG11 | 1.89                     | 0.54              |
| 24:K:157:ARG:NE    | 27:N:43:GLU:O      | 2.40                     | 0.54              |
| 25:L:39:LEU:HB3    | 25:L:62:MET:HE1    | 1.88                     | 0.54              |
| 26:M:79:ARG:O      | 26:M:79:ARG:HD2    | 2.06                     | 0.54              |
| 26:M:103:TRP:HB3   | 26:M:137:LYS:HD3   | 1.89                     | 0.54              |
| 27:N:50:LYS:HE2    | 27:N:50:LYS:HA     | 1.89                     | 0.54              |
| 28:O:88:MET:HE1    | 28:O:95:ARG:HA     | 1.89                     | 0.54              |
| 40:a:2191:A:H2'    | 40:a:2192:U:H6     | 1.71                     | 0.54              |
| 40:a:2356:U:H4'    | 41:b:20:ARG:HH11   | 1.72                     | 0.54              |
| 40:a:2838:G:C4     | 40:a:2839:G:C8     | 2.95                     | 0.54              |
| 64:y:31:TRP:CZ3    | 64:y:40:LEU:HD11   | 2.43                     | 0.54              |
| 2:1:25:ARG:NH2     | 40:a:519:U:O3'     | 2.40                     | 0.54              |
| 5:4:57:TYR:HB3     | 61:v:136:MET:HE3   | 1.87                     | 0.54              |
| 9:9:31:ARG:CD      | 40:a:1053:C:O2'    | 2.47                     | 0.54              |
| 11:AA:633:LEU:HD13 | 11:AA:644:LEU:HD23 | 1.89                     | 0.54              |
| 10:B:22:G:O2'      | 10:B:23:C:P        | 2.65                     | 0.54              |
| 10:B:60:U:P        | 10:B:61:C:H41      | 2.30                     | 0.54              |
| 16:C:34:THR:HG22   | 16:C:36:SER:H      | 1.72                     | 0.54              |
| 17:D:547:A:OP1     | 23:J:70:ARG:NH2    | 2.41                     | 0.54              |
| 22:I:164:ARG:CZ    | 22:I:166:GLU:OE2   | 2.54                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:J:162:ALA:HA    | 23:J:165:ARG:CZ    | 2.36                     | 0.54              |
| 24:K:14:LYS:HD3    | 24:K:117:VAL:CG1   | 2.38                     | 0.54              |
| 27:N:78:VAL:HG12   | 27:N:85:ILE:HG21   | 1.89                     | 0.54              |
| 40:a:1469:A:H2'    | 40:a:1470:A:C8     | 2.42                     | 0.54              |
| 40:a:1817:G:C6     | 40:a:1818:U:C5     | 2.95                     | 0.54              |
| 40:a:2741:A:O3'    | 56:q:36:ARG:NH1    | 2.40                     | 0.54              |
| 51:l:60:TRP:CD1    | 51:l:65:THR:HG21   | 2.43                     | 0.54              |
| 55:p:149:ARG:NE    | 55:p:162:VAL:O     | 2.40                     | 0.54              |
| 2:1:62:ASP:OD1     | 2:1:62:ASP:O       | 2.24                     | 0.54              |
| 9:9:73:LYS:HD2     | 9:9:73:LYS:O       | 2.06                     | 0.54              |
| 9:9:136:ILE:CD1    | 9:9:139:LEU:HD12   | 2.25                     | 0.54              |
| 11:AA:377:THR:HB   | 12:AB:65:HIS:NE2   | 2.23                     | 0.54              |
| 17:D:17:U:H2'      | 17:D:18:C:C6       | 2.42                     | 0.54              |
| 17:D:73:C:O2       | 17:D:73:C:H2'      | 2.07                     | 0.54              |
| 26:M:23:LEU:O      | 26:M:27:VAL:HG13   | 2.07                     | 0.54              |
| 29:P:5:ARG:HG3     | 29:P:7:ARG:NH1     | 2.23                     | 0.54              |
| 40:a:1019:U:O4     | 40:a:1142:A:N1     | 2.40                     | 0.54              |
| 40:a:1266:G:OP1    | 48:i:16:ARG:NE     | 2.35                     | 0.54              |
| 40:a:1353:A:H2'    | 40:a:1354:A:C8     | 2.43                     | 0.54              |
| 40:a:2297:A:C2     | 40:a:2320:U:O4'    | 2.61                     | 0.54              |
| 40:a:2376:A:N3     | 63:x:111:ARG:NH1   | 2.54                     | 0.54              |
| 47:h:107:PRO:HD2   | 47:h:110:LEU:HD22  | 1.89                     | 0.54              |
| 51:l:175:ILE:CG2   | 51:l:180:LEU:HD11  | 2.38                     | 0.54              |
| 53:n:5:HIS:HD2     | 53:n:97:TRP:CE2    | 2.24                     | 0.54              |
| 57:r:33:GLN:HB3    | 57:r:35:LYS:HZ3    | 1.72                     | 0.54              |
| 58:s:74:TYR:CE2    | 58:s:92:MET:HE1    | 2.42                     | 0.54              |
| 62:w:94:TYR:C      | 62:w:116:VAL:HG23  | 2.32                     | 0.54              |
| 4:3:7:ARG:HB3      | 40:a:85:G:OP2      | 2.07                     | 0.54              |
| 7:6:20:DA:N6       | 8:7:33:G:C2        | 2.76                     | 0.54              |
| 9:9:94:ARG:CB      | 9:9:97:LYS:HZ3     | 2.19                     | 0.54              |
| 11:AA:143:ARG:NH2  | 11:AA:512:SER:O    | 2.40                     | 0.54              |
| 12:AB:141:LEU:CA   | 12:AB:152:HIS:C    | 2.80                     | 0.54              |
| 13:AC:100:LEU:HD23 | 13:AC:115:ILE:HG21 | 1.89                     | 0.54              |
| 17:D:280:C:H1'     | 35:V:40:ARG:CZ     | 2.37                     | 0.54              |
| 17:D:564:C:P       | 31:R:12:ARG:HH22   | 2.30                     | 0.54              |
| 17:D:695:A:OP1     | 30:Q:53:ARG:HD3    | 2.07                     | 0.54              |
| 19:F:63:GLU:HG2    | 19:F:67:ARG:NH2    | 2.23                     | 0.54              |
| 22:I:132:ARG:HA    | 22:I:135:LYS:HE3   | 1.89                     | 0.54              |
| 23:J:175:ALA:O     | 23:J:178:MET:SD    | 2.65                     | 0.54              |
| 24:K:131:THR:O     | 24:K:131:THR:HG22  | 2.08                     | 0.54              |
| 40:a:3:U:H2'       | 40:a:4:U:C6        | 2.43                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:a:728:G:C4     | 40:a:730:A:C8      | 2.95                     | 0.54              |
| 40:a:1000:A:H2'   | 40:a:1001:A:C8     | 2.42                     | 0.54              |
| 40:a:2833:U:O2    | 49:j:58:ASN:ND2    | 2.41                     | 0.54              |
| 46:g:61:ASN:OD1   | 46:g:65:ASN:ND2    | 2.40                     | 0.54              |
| 50:k:5:ILE:HG23   | 50:k:28:ARG:NH1    | 2.21                     | 0.54              |
| 53:n:134:GLU:N    | 53:n:134:GLU:OE1   | 2.40                     | 0.54              |
| 57:r:143:ILE:O    | 57:r:143:ILE:HG13  | 2.08                     | 0.54              |
| 1:0:10:LYS:CE     | 40:a:996:A:OP1     | 2.56                     | 0.54              |
| 5:4:35:GLU:OE1    | 5:4:93:ARG:CZ      | 2.56                     | 0.54              |
| 8:7:3:G:C3'       | 17:D:1500:A:N6     | 2.71                     | 0.54              |
| 9:9:36:ASP:N      | 9:9:36:ASP:OD1     | 2.40                     | 0.54              |
| 9:9:61:ARG:NH2    | 40:a:1045:C:O3'    | 2.40                     | 0.54              |
| 9:9:129:LEU:HD12  | 9:9:129:LEU:C      | 2.32                     | 0.54              |
| 10:A:18:G:H1'     | 10:A:58:A:C2       | 2.41                     | 0.54              |
| 14:AE:1346:GLY:O  | 14:AE:1350:ASN:ND2 | 2.41                     | 0.54              |
| 16:C:60:LYS:HD2   | 17:D:734:G:O2'     | 2.07                     | 0.54              |
| 18:E:25:ARG:HD3   | 18:E:66:LEU:HD11   | 1.90                     | 0.54              |
| 19:F:31:GLU:O     | 19:F:34:ARG:HG2    | 2.08                     | 0.54              |
| 21:H:118:GLY:O    | 21:H:133:GLY:HA2   | 2.06                     | 0.54              |
| 33:T:3:LEU:HD22   | 33:T:8:THR:HG22    | 1.88                     | 0.54              |
| 38:Y:45:THR:HG21  | 38:Y:50:LYS:CD     | 2.36                     | 0.54              |
| 40:a:16:C:O4'     | 48:i:15:MET:CE     | 2.55                     | 0.54              |
| 40:a:1563:U:H2'   | 40:a:1564:C:C6     | 2.43                     | 0.54              |
| 40:a:2020:A:C2    | 40:a:2022:U:O4'    | 2.61                     | 0.54              |
| 40:a:2638:G:O2'   | 40:a:2775:G:N2     | 2.37                     | 0.54              |
| 59:t:73:ASP:OD2   | 64:y:80:VAL:HG11   | 2.08                     | 0.54              |
| 2:1:33:LEU:HD23   | 2:1:51:LEU:HD23    | 1.89                     | 0.54              |
| 5:4:6:ALA:HB3     | 5:4:65:VAL:CG2     | 2.37                     | 0.54              |
| 7:6:20:DA:C6      | 8:7:33:G:N2        | 2.76                     | 0.54              |
| 11:AA:684:ASN:OD1 | 11:AA:687:ARG:NH2  | 2.41                     | 0.54              |
| 12:AB:5:TYR:HA    | 12:AB:88:VAL:HG22  | 1.90                     | 0.54              |
| 17:D:106:C:N4     | 18:E:10:ARG:NH2    | 2.56                     | 0.54              |
| 18:E:24:ARG:O     | 18:E:28:MET:HG2    | 2.08                     | 0.54              |
| 20:G:19:GLN:CD    | 21:H:76:GLU:HB3    | 2.33                     | 0.54              |
| 24:K:112:ARG:HG3  | 24:K:116:GLU:OE2   | 2.06                     | 0.54              |
| 31:R:74:LEU:HD11  | 31:R:80:ILE:HD11   | 1.90                     | 0.54              |
| 40:a:151:C:C2     | 40:a:152:A:C8      | 2.95                     | 0.54              |
| 40:a:537:G:OP2    | 58:s:2:LYS:CE      | 2.55                     | 0.54              |
| 40:a:1082:U:O4    | 40:a:1086:A:N1     | 2.39                     | 0.54              |
| 40:a:1656:C:OP1   | 49:j:141:ARG:CD    | 2.56                     | 0.54              |
| 55:p:85:LYS:CE    | 55:p:164:TYR:CD1   | 2.86                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 60:u:57:LEU:HA    | 60:u:60:ARG:HD2   | 1.89                     | 0.54              |
| 61:v:97:GLN:H     | 61:v:100:LYS:CE   | 2.21                     | 0.54              |
| 61:v:111:GLU:OE1  | 61:v:111:GLU:N    | 2.32                     | 0.54              |
| 9:9:3:LEU:HD12    | 9:9:4:ASN:CA      | 2.37                     | 0.54              |
| 10:B:31:G:O2'     | 17:D:1340:A:H4'   | 2.08                     | 0.54              |
| 10:B:32:C:H5'     | 17:D:1340:A:O3'   | 2.06                     | 0.54              |
| 17:D:679:C:C2     | 17:D:680:C:C5     | 2.95                     | 0.54              |
| 18:E:19:LYS:HG3   | 18:E:20:HIS:N     | 2.22                     | 0.54              |
| 21:H:279:LYS:HA   | 21:H:331:MET:HB3  | 1.90                     | 0.54              |
| 21:H:332:VAL:HG12 | 21:H:334:ASP:H    | 1.73                     | 0.54              |
| 23:J:61:VAL:HG21  | 23:J:200:ILE:HD11 | 1.90                     | 0.54              |
| 24:K:77:ASN:HB2   | 24:K:82:GLN:HG3   | 1.89                     | 0.54              |
| 25:L:3:HIS:CG     | 25:L:65:GLU:OE1   | 2.61                     | 0.54              |
| 25:L:39:LEU:O     | 25:L:39:LEU:HD12  | 2.07                     | 0.54              |
| 32:S:42:TRP:CH2   | 46:g:66:ILE:HG23  | 2.42                     | 0.54              |
| 38:Y:32:VAL:HA    | 38:Y:60:VAL:HG21  | 1.90                     | 0.54              |
| 38:Y:77:VAL:O     | 38:Y:77:VAL:HG12  | 2.08                     | 0.54              |
| 40:a:839:U:H2'    | 40:a:840:C:H6     | 1.73                     | 0.54              |
| 40:a:1084:A:N7    | 40:a:1085:A:C6    | 2.76                     | 0.54              |
| 40:a:1830:C:C2    | 40:a:1831:G:C8    | 2.96                     | 0.54              |
| 40:a:2002:G:OP1   | 62:w:17:ARG:NH2   | 2.26                     | 0.54              |
| 40:a:2064:C:H2'   | 40:a:2065:C:C6    | 2.42                     | 0.54              |
| 40:a:2649:C:H2'   | 40:a:2650:U:H6    | 1.73                     | 0.54              |
| 44:e:28:LEU:HD23  | 44:e:43:LEU:HD22  | 1.88                     | 0.54              |
| 49:j:4:LEU:HG     | 49:j:32:ASN:OD1   | 2.08                     | 0.54              |
| 59:t:2:ILE:CG2    | 59:t:8:LEU:HD11   | 2.38                     | 0.54              |
| 59:t:41:ILE:HD11  | 59:t:86:LEU:HD22  | 1.89                     | 0.54              |
| 6:5:16:DG:OP1     | 11:AA:175:ARG:NH2 | 2.39                     | 0.54              |
| 16:C:13:PHE:CZ    | 16:C:21:ILE:HG12  | 2.42                     | 0.54              |
| 17:D:399:G:H2'    | 17:D:400:C:C6     | 2.43                     | 0.54              |
| 17:D:662:U:O2'    | 17:D:836:G:OP1    | 2.21                     | 0.54              |
| 22:I:85:GLU:HG3   | 22:I:89:LYS:NZ    | 2.23                     | 0.54              |
| 27:N:87:LYS:HG2   | 27:N:92:LEU:HA    | 1.90                     | 0.54              |
| 31:R:56:ARG:HA    | 31:R:62:GLU:OE2   | 2.08                     | 0.54              |
| 35:V:31:HIS:ND1   | 35:V:32:PRO:HD2   | 2.23                     | 0.54              |
| 38:Y:44:LYS:O     | 38:Y:44:LYS:HD2   | 2.07                     | 0.54              |
| 40:a:134:G:H2'    | 40:a:135:U:C6     | 2.43                     | 0.54              |
| 40:a:581:C:H2'    | 40:a:582:A:H8     | 1.73                     | 0.54              |
| 40:a:2063:C:O2    | 40:a:2063:C:H2'   | 2.07                     | 0.54              |
| 53:n:16:LEU:HD11  | 53:n:169:LEU:CD1  | 2.38                     | 0.54              |
| 60:u:76:GLU:CG    | 60:u:111:ILE:HD13 | 2.37                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:z:78:LYS:CD     | 65:z:117:LEU:CD2   | 2.84                     | 0.54              |
| 9:9:97:LYS:HD3     | 9:9:130:PRO:HG3    | 1.89                     | 0.54              |
| 9:9:98:GLU:HA      | 9:9:101:LYS:HZ3    | 1.72                     | 0.54              |
| 11:AA:29:SER:O     | 11:AA:33:ASP:HB2   | 2.07                     | 0.54              |
| 17:D:37:U:O4       | 17:D:397:A:N1      | 2.40                     | 0.54              |
| 17:D:197:A:H1'     | 17:D:198:G:OP2     | 2.08                     | 0.54              |
| 17:D:1399:C:O2     | 17:D:1502:A:N6     | 2.40                     | 0.54              |
| 18:E:9:LYS:C       | 18:E:13:GLN:NE2    | 2.62                     | 0.54              |
| 24:K:86:LYS:N      | 24:K:86:LYS:HD2    | 2.23                     | 0.54              |
| 26:M:31:MET:SD     | 26:M:36:LYS:HA     | 2.48                     | 0.54              |
| 38:Y:80:LYS:CG     | 38:Y:86:LYS:O      | 2.56                     | 0.54              |
| 40:a:588:U:H2'     | 40:a:589:U:C6      | 2.43                     | 0.54              |
| 40:a:2308:G:C5     | 53:n:77:PHE:HZ     | 2.26                     | 0.54              |
| 40:a:2454:G:C4     | 40:a:2455:G:C8     | 2.96                     | 0.54              |
| 47:h:74:ILE:CG2    | 47:h:96:TYR:HD1    | 2.21                     | 0.54              |
| 58:s:133:ALA:C     | 58:s:135:GLN:H     | 2.16                     | 0.54              |
| 59:t:14:SER:OG     | 59:t:86:LEU:HD12   | 2.08                     | 0.54              |
| 63:x:48:LEU:CD2    | 63:x:87:ILE:HD11   | 2.38                     | 0.54              |
| 64:y:27:GLU:HB3    | 64:y:87:LYS:NZ     | 2.22                     | 0.54              |
| 1:0:13:ARG:NH2     | 65:z:97:ASP:OD1    | 2.40                     | 0.54              |
| 6:5:9:DG:H2'       | 12:AB:71:ALA:HA    | 1.90                     | 0.54              |
| 9:9:3:LEU:CG       | 9:9:4:ASN:H        | 2.21                     | 0.54              |
| 12:AB:36:GLU:H     | 12:AB:106:ASP:CG   | 2.15                     | 0.54              |
| 14:AE:1175:LEU:O   | 14:AE:1187:GLU:HA  | 2.08                     | 0.54              |
| 17:D:76:G:C4       | 17:D:77:A:C8       | 2.95                     | 0.54              |
| 18:E:56:PRO:HG2    | 18:E:57:ILE:HD12   | 1.90                     | 0.54              |
| 20:G:148:LEU:HD22  | 20:G:151:ILE:HD11  | 1.89                     | 0.54              |
| 25:L:42:TRP:CZ2    | 25:L:102:MET:SD    | 3.01                     | 0.54              |
| 29:P:6:ILE:HG21    | 29:P:100:ILE:HD11  | 1.89                     | 0.54              |
| 30:Q:79:ILE:O      | 30:Q:105:PHE:HE1   | 1.91                     | 0.54              |
| 38:Y:33:ASN:HB2    | 38:Y:36:GLU:OE2    | 2.08                     | 0.54              |
| 38:Y:77:VAL:HG13   | 38:Y:81:LYS:HZ3    | 1.73                     | 0.54              |
| 40:a:2351:G:O6     | 54:o:39:LYS:CE     | 2.55                     | 0.54              |
| 40:a:2747:G:O6     | 40:a:2755:C:H5''   | 2.08                     | 0.54              |
| 44:e:4:LYS:HZ2     | 44:e:7:ARG:HH12    | 1.55                     | 0.54              |
| 63:x:38:GLN:HG2    | 63:x:50:ALA:CB     | 2.38                     | 0.54              |
| 3:2:30:ILE:HG22    | 3:2:32:LEU:CD2     | 2.38                     | 0.53              |
| 14:AE:1000:GLY:HA3 | 14:AE:1026:PRO:HG2 | 1.90                     | 0.53              |
| 17:D:1329:A:P      | 37:X:28:THR:HB     | 2.48                     | 0.53              |
| 17:D:1358:U:O4     | 17:D:1363:A:N1     | 2.41                     | 0.53              |
| 18:E:25:ARG:HD3    | 18:E:66:LEU:HD21   | 1.90                     | 0.53              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 27:N:83:LEU:HD21   | 31:R:4:VAL:HG11     | 1.89                     | 0.53              |
| 27:N:87:LYS:HD2    | 27:N:91:GLU:CB      | 2.37                     | 0.53              |
| 28:O:67:VAL:C      | 28:O:68:LYS:HD2     | 2.33                     | 0.53              |
| 31:R:25:GLU:OE1    | 31:R:59:ASN:ND2     | 2.42                     | 0.53              |
| 37:X:96:PRO:HG3    | 37:X:102:THR:HG22   | 1.89                     | 0.53              |
| 40:a:151:C:H2'     | 40:a:152:A:H8       | 1.72                     | 0.53              |
| 40:a:1386:C:H2'    | 40:a:1387:A:C8      | 2.42                     | 0.53              |
| 40:a:2038:G:H2'    | 40:a:2039:U:O4'     | 2.08                     | 0.53              |
| 40:a:2259:U:C2     | 40:a:2260:C:C6      | 2.96                     | 0.53              |
| 49:j:55:LYS:HZ1    | 49:j:60:VAL:N       | 2.06                     | 0.53              |
| 53:n:71:ARG:O      | 53:n:81:GLN:NE2     | 2.40                     | 0.53              |
| 58:s:15:TRP:HE3    | 58:s:135:GLN:O      | 1.90                     | 0.53              |
| 61:v:45:GLN:NE2    | 61:v:125:PRO:HD2    | 2.23                     | 0.53              |
| 2:1:41:LYS:HE3     | 40:a:2010:G:P       | 2.48                     | 0.53              |
| 3:2:56:GLU:OE1     | 3:2:87:LEU:CA       | 2.56                     | 0.53              |
| 8:7:19:U:H3'       | 8:7:19:U:H6         | 1.73                     | 0.53              |
| 12:AB:119:THR:HA   | 12:AB:125:GLY:H     | 1.73                     | 0.53              |
| 25:L:62:MET:HA     | 25:L:62:MET:HE3     | 1.90                     | 0.53              |
| 26:M:103:TRP:CD1   | 26:M:137:LYS:HZ2    | 2.25                     | 0.53              |
| 37:X:81:MET:CE     | 37:X:92:ARG:HD3     | 2.38                     | 0.53              |
| 38:Y:116:MET:HG2   | 38:Y:124:MET:HB3    | 1.91                     | 0.53              |
| 40:a:2766:A:C2     | 40:a:2767:C:C6      | 2.95                     | 0.53              |
| 47:h:17:VAL:HB     | 47:h:204:VAL:HG12   | 1.89                     | 0.53              |
| 49:j:124:ARG:NH1   | 49:j:161:MET:O      | 2.41                     | 0.53              |
| 60:u:111:ILE:HD12  | 60:u:111:ILE:N      | 2.23                     | 0.53              |
| 61:v:21:ALA:HB2    | 61:v:100:LYS:HG3    | 1.90                     | 0.53              |
| 61:v:45:GLN:HE21   | 61:v:124:LEU:HD23   | 1.72                     | 0.53              |
| 65:z:92:ARG:HA     | 65:z:95:LEU:HD12    | 1.89                     | 0.53              |
| 2:1:31:GLN:O       | 2:1:35:ILE:HG12     | 2.07                     | 0.53              |
| 4:3:26:LYS:HE3     | 4:3:37:GLU:HB2      | 1.90                     | 0.53              |
| 12:AB:121:GLY:HA3  | 12:AB:162:LEU:CD1   | 2.33                     | 0.53              |
| 14:AE:886:VAL:HG11 | 14:AE:1230:THR:HG21 | 1.89                     | 0.53              |
| 17:D:750:C:C2      | 17:D:751:U:C5       | 2.96                     | 0.53              |
| 18:E:22:ALA:CA     | 18:E:25:ARG:HH21    | 2.21                     | 0.53              |
| 20:G:58:ASN:OD1    | 20:G:223:GLU:OE1    | 2.26                     | 0.53              |
| 21:H:71:ALA:C      | 21:H:72:LEU:HD12    | 2.32                     | 0.53              |
| 22:I:85:GLU:O      | 22:I:89:LYS:HE2     | 2.08                     | 0.53              |
| 28:O:5:GLN:NE2     | 28:O:22:LYS:NZ      | 2.56                     | 0.53              |
| 28:O:10:GLY:HA3    | 28:O:78:ALA:O       | 2.08                     | 0.53              |
| 40:a:1412:U:C4     | 40:a:1413:A:N7      | 2.77                     | 0.53              |
| 40:a:2387:U:O4'    | 41:b:41:ARG:NH1     | 2.41                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:h:123:ALA:HB1   | 47:h:125:LYS:HZ1   | 1.74                     | 0.53              |
| 55:p:89:LEU:HD22   | 55:p:162:VAL:HG22  | 1.91                     | 0.53              |
| 59:t:1:MET:CE      | 59:t:32:TYR:CB     | 2.87                     | 0.53              |
| 62:w:44:LEU:HD22   | 62:w:113:ILE:HD13  | 1.90                     | 0.53              |
| 1:0:10:LYS:CE      | 40:a:994:C:O2'     | 2.56                     | 0.53              |
| 3:2:6:ARG:NH2      | 3:2:10:VAL:HG22    | 2.24                     | 0.53              |
| 7:6:14:DC:H2'      | 7:6:15:DC:C6       | 2.43                     | 0.53              |
| 8:7:13:U:H6        | 8:7:13:U:H5''      | 1.73                     | 0.53              |
| 11:AA:243:PRO:HB2  | 11:AA:274:ILE:HG23 | 1.90                     | 0.53              |
| 17:D:736:C:H2'     | 17:D:737:C:C6      | 2.43                     | 0.53              |
| 18:E:32:ILE:CG2    | 18:E:75:HIS:NE2    | 2.71                     | 0.53              |
| 24:K:137:VAL:O     | 24:K:141:ILE:HG12  | 2.09                     | 0.53              |
| 25:L:36:ILE:O      | 25:L:36:ILE:HG23   | 2.08                     | 0.53              |
| 26:M:4:ARG:HG3     | 26:M:5:ARG:CG      | 2.22                     | 0.53              |
| 31:R:110:ARG:NE    | 31:R:117:TYR:CD2   | 2.76                     | 0.53              |
| 40:a:1779:U:H5     | 40:a:1784:A:N7     | 2.06                     | 0.53              |
| 51:l:60:TRP:NE1    | 51:l:69:ARG:HH12   | 2.07                     | 0.53              |
| 55:p:33:LEU:HD11   | 55:p:136:ALA:HB1   | 1.89                     | 0.53              |
| 61:v:97:GLN:N      | 61:v:100:LYS:CE    | 2.72                     | 0.53              |
| 5:4:80:HIS:ND1     | 5:4:83:LYS:HB2     | 2.23                     | 0.53              |
| 6:5:9:DG:OP2       | 11:AA:473:ARG:HG2  | 2.05                     | 0.53              |
| 13:AC:43:LEU:HD13  | 13:AC:217:ILE:HD11 | 1.90                     | 0.53              |
| 14:AE:526:VAL:HG12 | 14:AE:549:LYS:HB2  | 1.90                     | 0.53              |
| 16:C:54:GLN:HG3    | 16:C:55:LEU:N      | 2.22                     | 0.53              |
| 17:D:769:G:H4'     | 17:D:1513:A:H4'    | 1.90                     | 0.53              |
| 20:G:18:HIS:HA     | 21:H:43:LYS:HD2    | 1.90                     | 0.53              |
| 20:G:53:ALA:CA     | 20:G:56:GLU:OE1    | 2.57                     | 0.53              |
| 26:M:85:TYR:CD2    | 26:M:151:PHE:CZ    | 2.96                     | 0.53              |
| 29:P:27:GLU:HA     | 29:P:30:LYS:NZ     | 2.23                     | 0.53              |
| 30:Q:20:VAL:HB     | 30:Q:35:THR:HG23   | 1.89                     | 0.53              |
| 31:R:35:THR:OG1    | 31:R:56:ARG:HG3    | 2.08                     | 0.53              |
| 33:T:11:ILE:HA     | 33:T:14:GLU:OE1    | 2.09                     | 0.53              |
| 37:X:28:THR:CA     | 37:X:31:LYS:HE3    | 2.37                     | 0.53              |
| 40:a:998:C:OP1     | 65:z:84:LYS:NZ     | 2.39                     | 0.53              |
| 40:a:1278:C:H5'    | 62:w:24:MET:SD     | 2.49                     | 0.53              |
| 40:a:1348:C:C4     | 40:a:1349:C:C6     | 2.97                     | 0.53              |
| 40:a:1657:U:O2'    | 49:j:138:LEU:HD22  | 2.08                     | 0.53              |
| 40:a:1790:C:H2'    | 40:a:1791:A:C5     | 2.43                     | 0.53              |
| 40:a:1820:U:C4     | 47:h:159:GLY:HA3   | 2.44                     | 0.53              |
| 40:a:2849:U:O5'    | 64:y:93:ARG:NH2    | 2.42                     | 0.53              |
| 46:g:47:LYS:HD3    | 53:n:178:ARG:HH22  | 1.73                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 49:j:48:ILE:HG12  | 49:j:84:LEU:HD21   | 1.91                     | 0.53              |
| 50:k:29:THR:HG23  | 50:k:30:LYS:HG2    | 1.90                     | 0.53              |
| 53:n:72:LYS:HA    | 53:n:81:GLN:HE22   | 1.74                     | 0.53              |
| 53:n:94:GLU:HA    | 53:n:97:TRP:CE3    | 2.43                     | 0.53              |
| 59:t:18:ARG:HB3   | 59:t:45:GLU:HB3    | 1.89                     | 0.53              |
| 61:v:96:ILE:HA    | 61:v:100:LYS:CE    | 2.38                     | 0.53              |
| 8:7:3:G:H3'       | 17:D:1500:A:N6     | 2.24                     | 0.53              |
| 10:A:41:C:O4'     | 26:M:143:ARG:NH1   | 2.41                     | 0.53              |
| 12:AB:27:ASN:ND2  | 12:AB:58:GLU:HB2   | 2.24                     | 0.53              |
| 13:AD:28:LEU:HD12 | 13:AD:201:LEU:HD23 | 1.90                     | 0.53              |
| 14:AE:122:SER:HB2 | 14:AE:132:LEU:HD12 | 1.91                     | 0.53              |
| 15:AF:3:ARG:NH1   | 15:AF:55:GLU:OE2   | 2.40                     | 0.53              |
| 10:B:38:A:O2'     | 17:D:790:A:O5'     | 2.27                     | 0.53              |
| 17:D:274:A:H4'    | 35:V:16:LYS:NZ     | 2.24                     | 0.53              |
| 22:I:142:MET:SD   | 22:I:170:GLU:OE1   | 2.67                     | 0.53              |
| 23:J:105:MET:HE1  | 23:J:171:LEU:HB3   | 1.89                     | 0.53              |
| 26:M:79:ARG:HB2   | 26:M:84:THR:HG23   | 1.90                     | 0.53              |
| 29:P:47:GLU:OE1   | 29:P:67:ILE:HG23   | 2.08                     | 0.53              |
| 30:Q:84:VAL:HG21  | 30:Q:97:ILE:CD1    | 2.39                     | 0.53              |
| 30:Q:86:VAL:O     | 30:Q:113:VAL:HG22  | 2.08                     | 0.53              |
| 36:W:66:MET:HG2   | 36:W:74:PHE:CZ     | 2.44                     | 0.53              |
| 38:Y:77:VAL:HA    | 38:Y:80:LYS:HD3    | 1.91                     | 0.53              |
| 40:a:67:U:N3      | 40:a:74:A:C6       | 2.77                     | 0.53              |
| 40:a:1266:G:O2'   | 40:a:2012:G:O6     | 2.22                     | 0.53              |
| 40:a:2328:A:H2'   | 40:a:2329:U:H6     | 1.68                     | 0.53              |
| 51:l:62:GLN:O     | 51:l:69:ARG:CD     | 2.56                     | 0.53              |
| 51:l:69:ARG:HA    | 51:l:69:ARG:CZ     | 2.37                     | 0.53              |
| 53:n:42:GLU:HG3   | 53:n:49:LEU:HD23   | 1.91                     | 0.53              |
| 53:n:46:ASP:CG    | 53:n:49:LEU:HD13   | 2.33                     | 0.53              |
| 5:4:19:ARG:NH1    | 43:d:95:U:OP2      | 2.41                     | 0.53              |
| 5:4:35:GLU:OE1    | 5:4:36:ALA:O       | 2.27                     | 0.53              |
| 6:5:10:DT:C7      | 11:AA:62:TYR:HB3   | 2.37                     | 0.53              |
| 9:9:52:MET:HE1    | 9:9:85:SER:CA      | 2.38                     | 0.53              |
| 14:AE:66:LYS:HB2  | 14:AE:69:GLU:CB    | 2.38                     | 0.53              |
| 17:D:1308:U:H3'   | 37:X:98:ARG:CZ     | 2.39                     | 0.53              |
| 22:I:49:LYS:NZ    | 22:I:75:ILE:HD11   | 2.24                     | 0.53              |
| 38:Y:102:ARG:HG3  | 38:Y:140:GLU:C     | 2.33                     | 0.53              |
| 40:a:372:G:O2'    | 42:c:54:LYS:HE3    | 2.09                     | 0.53              |
| 52:m:25:LYS:HG3   | 52:m:29:GLN:HE22   | 1.73                     | 0.53              |
| 62:w:14:SER:HA    | 62:w:17:ARG:CZ     | 2.39                     | 0.53              |
| 3:2:53:VAL:HG21   | 3:2:87:LEU:HD23    | 1.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AA:360:LEU:HD13 | 11:AA:378:ARG:HH11 | 1.72                     | 0.53              |
| 12:AB:123:PHE:CE2  | 29:P:81:GLU:C      | 2.87                     | 0.53              |
| 14:AE:77:ARG:HD3   | 14:AE:78:LEU:H     | 1.73                     | 0.53              |
| 14:AE:514:THR:HG21 | 14:AE:596:LEU:HD12 | 1.90                     | 0.53              |
| 16:C:12:ARG:NH2    | 16:C:13:PHE:CE1    | 2.77                     | 0.53              |
| 16:C:40:VAL:HG13   | 21:H:339:ARG:HD3   | 1.89                     | 0.53              |
| 17:D:552:U:O2'     | 31:R:83:ARG:O      | 2.19                     | 0.53              |
| 26:M:4:ARG:CG      | 26:M:5:ARG:NH1     | 2.72                     | 0.53              |
| 39:Z:18:ASP:HB3    | 39:Z:22:LEU:CD1    | 2.39                     | 0.53              |
| 40:a:813:U:H2'     | 40:a:814:C:H6      | 1.74                     | 0.53              |
| 40:a:1295:C:C2     | 40:a:1296:G:C8     | 2.97                     | 0.53              |
| 40:a:2473:U:O2     | 40:a:2473:U:H2'    | 2.09                     | 0.53              |
| 40:a:2847:U:H2'    | 40:a:2848:G:O4'    | 2.08                     | 0.53              |
| 53:n:93:GLY:HA2    | 53:n:97:TRP:CZ3    | 2.44                     | 0.53              |
| 53:n:132:VAL:CG2   | 53:n:152:LEU:HD23  | 2.39                     | 0.53              |
| 59:t:1:MET:CE      | 59:t:32:TYR:HB3    | 2.38                     | 0.53              |
| 60:u:54:GLN:NE2    | 60:u:60:ARG:HH12   | 2.07                     | 0.53              |
| 1:0:4:VAL:HG22     | 1:0:40:MET:HB3     | 1.91                     | 0.53              |
| 9:9:24:SER:HG      | 9:9:85:SER:C       | 2.17                     | 0.53              |
| 11:AA:481:LEU:CD2  | 12:AB:16:ARG:HD2   | 2.12                     | 0.53              |
| 10:B:38:A:O2'      | 17:D:790:A:P       | 2.66                     | 0.53              |
| 17:D:339:C:H2'     | 17:D:340:U:H6      | 1.73                     | 0.53              |
| 20:G:23:TRP:HB3    | 20:G:39:HIS:CE1    | 2.44                     | 0.53              |
| 22:I:58:GLU:OE2    | 22:I:60:PRO:HD3    | 2.08                     | 0.53              |
| 23:J:67:VAL:HB     | 23:J:72:PHE:CE1    | 2.43                     | 0.53              |
| 27:N:31:LYS:HE3    | 27:N:31:LYS:HA     | 1.90                     | 0.53              |
| 30:Q:20:VAL:HG13   | 30:Q:85:MET:HE1    | 1.89                     | 0.53              |
| 38:Y:78:LEU:HD13   | 38:Y:108:ILE:HG12  | 1.90                     | 0.53              |
| 40:a:78:U:H2'      | 40:a:79:C:C6       | 2.44                     | 0.53              |
| 40:a:414:C:H2'     | 40:a:415:A:C8      | 2.44                     | 0.53              |
| 40:a:537:G:P       | 58:s:2:LYS:HE2     | 2.49                     | 0.53              |
| 40:a:590:A:H2'     | 40:a:591:U:C6      | 2.44                     | 0.53              |
| 40:a:1167:C:C2     | 40:a:1168:G:C8     | 2.97                     | 0.53              |
| 40:a:1665:A:C3'    | 59:t:66:LYS:HZ2    | 2.22                     | 0.53              |
| 40:a:2356:U:C5'    | 41:b:20:ARG:HD2    | 2.36                     | 0.53              |
| 50:k:8:LYS:NZ      | 50:k:54:ILE:HG12   | 2.23                     | 0.53              |
| 52:m:26:ASN:O      | 52:m:30:VAL:HG23   | 2.08                     | 0.53              |
| 59:t:59:LYS:HZ3    | 59:t:92:GLU:HG2    | 1.74                     | 0.53              |
| 61:v:1:MET:HA      | 61:v:1:MET:CE      | 2.38                     | 0.53              |
| 65:z:78:LYS:HD3    | 65:z:117:LEU:HD23  | 1.88                     | 0.53              |
| 8:7:3:G:C4'        | 17:D:1500:A:H62    | 2.22                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:7:15:U:HI'       | 15:AF:83:VAL:HG11  | 1.91                     | 0.53              |
| 11:AA:811:ASN:HA   | 11:AA:815:SER:HB2  | 1.90                     | 0.53              |
| 12:AB:21:LEU:HB3   | 12:AB:26:VAL:CG1   | 2.38                     | 0.53              |
| 13:AD:16:ILE:HG23  | 13:AD:26:VAL:HG22  | 1.91                     | 0.53              |
| 19:F:17:ARG:HA     | 19:F:20:LYS:NZ     | 2.24                     | 0.53              |
| 22:I:24:ALA:C      | 22:I:29:PHE:CE2    | 2.87                     | 0.53              |
| 28:O:21:ILE:HD11   | 28:O:87:LEU:HD22   | 1.90                     | 0.53              |
| 30:Q:84:VAL:CG2    | 30:Q:107:ILE:HD11  | 2.37                     | 0.53              |
| 35:V:7:THR:CB      | 35:V:60:GLU:OE2    | 2.56                     | 0.53              |
| 38:Y:126:ARG:NH1   | 40:a:1082:U:C5'    | 2.72                     | 0.53              |
| 40:a:271:G:C4      | 40:a:272:A:N7      | 2.77                     | 0.53              |
| 40:a:1024:G:OP2    | 40:a:1025:G:O2'    | 2.25                     | 0.53              |
| 40:a:1818:U:C6     | 47:h:156:ARG:NH2   | 2.77                     | 0.53              |
| 45:f:10:THR:HB     | 45:f:56:LYS:NZ     | 2.22                     | 0.53              |
| 46:g:11:GLU:HA     | 46:g:25:ARG:HA     | 1.90                     | 0.53              |
| 49:j:4:LEU:HD23    | 49:j:29:VAL:HG11   | 1.89                     | 0.53              |
| 51:l:188:MET:HE2   | 51:l:193:VAL:HA    | 1.89                     | 0.53              |
| 53:n:29:PRO:HB2    | 53:n:169:LEU:HD22  | 1.91                     | 0.53              |
| 56:q:25:VAL:CB     | 56:q:35:GLN:OE1    | 2.56                     | 0.53              |
| 22:I:155:GLY:O     | 22:I:196:ILE:HG12  | 2.08                     | 0.52              |
| 36:W:47:LEU:O      | 36:W:62:VAL:HG23   | 2.09                     | 0.52              |
| 38:Y:16:MET:HG2    | 38:Y:16:MET:O      | 2.09                     | 0.52              |
| 40:a:1340:U:C5     | 40:a:1603:A:C8     | 2.97                     | 0.52              |
| 40:a:2315:G:O2'    | 53:n:125:ARG:HD3   | 2.09                     | 0.52              |
| 40:a:2867:G:C6     | 64:y:21:ARG:NH1    | 2.76                     | 0.52              |
| 51:l:60:TRP:NE1    | 51:l:69:ARG:NH1    | 2.57                     | 0.52              |
| 58:s:9:GLU:HG2     | 58:s:10:THR:HG23   | 1.90                     | 0.52              |
| 65:z:108:ALA:O     | 65:z:111:GLU:HG3   | 2.09                     | 0.52              |
| 2:1:24:ILE:O       | 2:1:71:VAL:HG21    | 2.08                     | 0.52              |
| 8:7:8:U:OP2        | 17:D:1397:C:C2     | 2.62                     | 0.52              |
| 8:7:9:U:C4         | 17:D:1196:A:C8     | 2.97                     | 0.52              |
| 11:AA:246:LEU:HB3  | 11:AA:269:ILE:HD13 | 1.91                     | 0.52              |
| 11:AA:1142:ARG:NH2 | 11:AA:1166:ASP:OD1 | 2.38                     | 0.52              |
| 12:AB:126:PHE:HE1  | 14:AE:87:LYS:HD3   | 1.74                     | 0.52              |
| 12:AB:129:ILE:N    | 12:AB:142:LEU:HB3  | 2.24                     | 0.52              |
| 13:AD:182:ARG:NH1  | 14:AE:534:GLU:OE1  | 2.42                     | 0.52              |
| 14:AE:1045:THR:O   | 14:AE:1067:ARG:NH2 | 2.41                     | 0.52              |
| 10:B:38:A:HO2'     | 17:D:790:A:P       | 2.30                     | 0.52              |
| 20:G:168:HIS:HB3   | 20:G:169:GLU:OE1   | 2.10                     | 0.52              |
| 23:J:50:ASP:O      | 23:J:53:VAL:HG22   | 2.09                     | 0.52              |
| 24:K:158:GLY:C     | 24:K:159:LYS:HD2   | 2.34                     | 0.52              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 26:M:27:VAL:HG12 | 26:M:43:VAL:HG21   | 1.90                     | 0.52              |
| 26:M:38:THR:O    | 26:M:42:ILE:HG12   | 2.08                     | 0.52              |
| 38:Y:9:LYS:CG    | 38:Y:55:PRO:HB3    | 2.39                     | 0.52              |
| 40:a:125:A:OP2   | 52:m:19:ARG:NH2    | 2.39                     | 0.52              |
| 40:a:1379:U:H4'  | 40:a:1380:G:OP1    | 2.09                     | 0.52              |
| 40:a:1801:A:OP2  | 47:h:146:MET:HE1   | 2.09                     | 0.52              |
| 40:a:2049:G:N2   | 49:j:161:MET:HE1   | 2.24                     | 0.52              |
| 49:j:131:ASP:OD2 | 49:j:132:ALA:N     | 2.42                     | 0.52              |
| 51:l:62:GLN:HA   | 51:l:69:ARG:HH21   | 1.74                     | 0.52              |
| 53:n:114:PHE:O   | 53:n:115:ARG:NE    | 2.34                     | 0.52              |
| 54:o:25:LYS:HB3  | 60:u:62:PRO:CG     | 2.40                     | 0.52              |
| 60:u:56:PRO:O    | 60:u:60:ARG:HG3    | 2.10                     | 0.52              |
| 61:v:115:GLU:O   | 61:v:119:LEU:HD23  | 2.10                     | 0.52              |
| 62:w:33:ILE:CD1  | 62:w:112:TYR:CD1   | 2.91                     | 0.52              |
| 2:1:61:ASN:OD1   | 40:a:496:G:H1'     | 2.08                     | 0.52              |
| 3:2:33:LYS:HG3   | 3:2:80:TRP:CE3     | 2.44                     | 0.52              |
| 14:AE:968:ASN:HA | 14:AE:1117:SER:HB2 | 1.90                     | 0.52              |
| 20:G:23:TRP:HZ3  | 20:G:25:PRO:CA     | 2.22                     | 0.52              |
| 20:G:127:ASP:O   | 20:G:128:LYS:HB3   | 2.09                     | 0.52              |
| 24:K:111:MET:HE2 | 24:K:125:ALA:HB1   | 1.90                     | 0.52              |
| 26:M:17:LYS:HZ2  | 26:M:18:PHE:HE1    | 1.54                     | 0.52              |
| 28:O:47:VAL:O    | 28:O:80:ARG:HD2    | 2.09                     | 0.52              |
| 28:O:112:GLU:HG3 | 28:O:115:LYS:HZ3   | 1.73                     | 0.52              |
| 32:S:79:LEU:HB2  | 32:S:84:VAL:HG22   | 1.91                     | 0.52              |
| 40:a:1666:G:OP1  | 59:t:66:LYS:HD3    | 2.10                     | 0.52              |
| 47:h:108:LYS:HD3 | 47:h:194:GLU:HB2   | 1.92                     | 0.52              |
| 49:j:131:ASP:OD1 | 49:j:134:HIS:HB2   | 2.10                     | 0.52              |
| 59:t:2:ILE:HG23  | 59:t:8:LEU:HD11    | 1.91                     | 0.52              |
| 61:v:20:LEU:H    | 61:v:20:LEU:HD23   | 1.73                     | 0.52              |
| 3:2:19:LYS:O     | 3:2:22:THR:OG1     | 2.22                     | 0.52              |
| 9:9:61:ARG:NE    | 40:a:1046:A:P      | 2.83                     | 0.52              |
| 17:D:932:C:C5'   | 26:M:4:ARG:HH11    | 2.22                     | 0.52              |
| 17:D:1208:C:H2'  | 17:D:1209:C:C6     | 2.40                     | 0.52              |
| 22:I:105:GLU:OE1 | 22:I:107:ARG:NE    | 2.42                     | 0.52              |
| 31:R:102:LEU:O   | 31:R:103:ASP:OD1   | 2.26                     | 0.52              |
| 32:S:54:ASP:HA   | 32:S:59:ARG:HD2    | 1.90                     | 0.52              |
| 40:a:617:G:C4'   | 51:l:199:MET:HE1   | 2.39                     | 0.52              |
| 40:a:995:C:N4    | 58:s:2:LYS:HG3     | 2.24                     | 0.52              |
| 40:a:1145:C:C2   | 40:a:1146:C:C5     | 2.97                     | 0.52              |
| 40:a:1145:C:N3   | 40:a:1146:C:C5     | 2.77                     | 0.52              |
| 40:a:2537:U:H2'  | 40:a:2538:C:C6     | 2.43                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 45:f:10:THR:HG23    | 45:f:11:ARG:HG2     | 1.90                     | 0.52              |
| 55:p:32:GLU:C       | 55:p:33:LEU:HD12    | 2.34                     | 0.52              |
| 58:s:15:TRP:CE3     | 58:s:135:GLN:O      | 2.63                     | 0.52              |
| 58:s:25:LEU:CD1     | 58:s:101:ILE:HD13   | 2.39                     | 0.52              |
| 2:1:27:LYS:O        | 2:1:71:VAL:HG22     | 2.10                     | 0.52              |
| 5:4:63:ILE:CD1      | 5:4:91:PHE:CD2      | 2.93                     | 0.52              |
| 9:9:93:ALA:O        | 9:9:129:LEU:O       | 2.27                     | 0.52              |
| 11:AA:524:ILE:HG21  | 11:AA:708:VAL:HG13  | 1.92                     | 0.52              |
| 12:AB:135:GLY:O     | 12:AB:137:ALA:N     | 2.43                     | 0.52              |
| 13:AD:205:MET:HE3   | 13:AD:213:PRO:HB3   | 1.90                     | 0.52              |
| 14:AE:342:LEU:HD23  | 14:AE:1352:ILE:HG23 | 1.90                     | 0.52              |
| 10:B:76:A:H1'       | 40:a:2494:G:P       | 2.50                     | 0.52              |
| 17:D:62:U:H2'       | 17:D:63:C:C6        | 2.44                     | 0.52              |
| 17:D:1175:G:N3      | 17:D:1176:A:C8      | 2.77                     | 0.52              |
| 33:T:3:LEU:HD22     | 33:T:8:THR:HG23     | 1.92                     | 0.52              |
| 38:Y:139:VAL:HG22   | 38:Y:140:GLU:N      | 2.25                     | 0.52              |
| 40:a:15:G:H2'       | 48:i:15:MET:HE1     | 1.90                     | 0.52              |
| 40:a:645:C:H2'      | 40:a:647:G:C8       | 2.45                     | 0.52              |
| 40:a:1009:A:OP2     | 58:s:39:LYS:NZ      | 2.37                     | 0.52              |
| 40:a:1204:A:O4'     | 40:a:1206:G:C8      | 2.63                     | 0.52              |
| 40:a:2822:G:O2'     | 40:a:2824:C:OP2     | 2.20                     | 0.52              |
| 47:h:52:ARG:NE      | 47:h:53:HIS:HE1     | 2.07                     | 0.52              |
| 50:k:21:TYR:CE2     | 50:k:49:TYR:CD2     | 2.98                     | 0.52              |
| 61:v:1:MET:CE       | 61:v:44:ARG:HA      | 2.38                     | 0.52              |
| 62:w:37:THR:OG1     | 62:w:40:LYS:CD      | 2.57                     | 0.52              |
| 8:7:21:U:H3'        | 8:7:21:U:H6         | 1.74                     | 0.52              |
| 9:9:55:VAL:HG12     | 9:9:56:ARG:N        | 2.25                     | 0.52              |
| 10:A:16:C:O2        | 40:a:2181:U:C5'     | 2.57                     | 0.52              |
| 11:AA:1287:LEU:HD13 | 14:AE:1357:ILE:HD11 | 1.91                     | 0.52              |
| 14:AE:679:TYR:OH    | 14:AE:754:ILE:O     | 2.23                     | 0.52              |
| 19:F:37:PHE:HB3     | 30:Q:124:PRO:O      | 2.10                     | 0.52              |
| 21:H:45:GLU:OE1     | 21:H:45:GLU:N       | 2.41                     | 0.52              |
| 22:I:142:MET:CE     | 22:I:170:GLU:OE1    | 2.58                     | 0.52              |
| 22:I:183:ASP:HB3    | 22:I:204:LYS:NZ     | 2.25                     | 0.52              |
| 23:J:74:ASN:O       | 23:J:77:LYS:HG2     | 2.10                     | 0.52              |
| 26:M:111:ARG:N      | 26:M:119:ARG:NH2    | 2.58                     | 0.52              |
| 33:T:15:PHE:CD2     | 33:T:30:ALA:CB      | 2.92                     | 0.52              |
| 33:T:63:ARG:HD2     | 33:T:67:LEU:CD2     | 2.40                     | 0.52              |
| 40:a:1416:G:HO2'    | 40:a:1417:C:P       | 2.32                     | 0.52              |
| 40:a:1818:U:O2'     | 47:h:153:GLN:O      | 2.23                     | 0.52              |
| 40:a:2093:G:OP2     | 57:r:22:LYS:HE3     | 2.09                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:a:2723:C:H4'    | 62:w:1:MET:HE3     | 1.92                     | 0.52              |
| 47:h:34:LEU:HD12   | 47:h:61:ALA:HB1    | 1.92                     | 0.52              |
| 51:l:170:ARG:CZ    | 51:l:176:ASP:OD1   | 2.58                     | 0.52              |
| 57:r:2:GLN:HG3     | 57:r:39:ALA:CB     | 2.40                     | 0.52              |
| 57:r:6:LEU:CD1     | 57:r:37:VAL:HG23   | 2.39                     | 0.52              |
| 59:t:38:ILE:HD11   | 59:t:112:PHE:CZ    | 2.43                     | 0.52              |
| 1:0:71:LYS:HG3     | 1:0:73:LYS:HE3     | 1.91                     | 0.52              |
| 7:6:19:DC:H2'      | 7:6:20:DA:H8       | 1.74                     | 0.52              |
| 13:AD:100:LEU:HD21 | 13:AD:121:VAL:HG11 | 1.90                     | 0.52              |
| 17:D:73:C:O2       | 17:D:73:C:C2'      | 2.57                     | 0.52              |
| 17:D:1240:U:C5     | 26:M:116:MET:HE2   | 2.44                     | 0.52              |
| 27:N:79:SER:HB2    | 27:N:85:ILE:HG22   | 1.92                     | 0.52              |
| 28:O:57:MET:HA     | 28:O:60:LYS:CE     | 2.40                     | 0.52              |
| 30:Q:61:PHE:CD1    | 30:Q:64:GLN:NE2    | 2.78                     | 0.52              |
| 37:X:96:PRO:CG     | 37:X:102:THR:HG22  | 2.40                     | 0.52              |
| 38:Y:58:ILE:HG23   | 38:Y:66:PHE:CD2    | 2.44                     | 0.52              |
| 38:Y:78:LEU:HD12   | 38:Y:112:LYS:NZ    | 2.25                     | 0.52              |
| 38:Y:129:GLU:CB    | 38:Y:133:ARG:HH12  | 2.16                     | 0.52              |
| 40:a:2355:G:H2'    | 40:a:2356:U:H5'    | 1.90                     | 0.52              |
| 40:a:2649:C:C2     | 40:a:2650:U:C5     | 2.97                     | 0.52              |
| 40:a:2727:A:O2'    | 59:t:70:ARG:NH2    | 2.43                     | 0.52              |
| 40:a:2758:A:H1'    | 55:p:38:ASN:HD21   | 1.74                     | 0.52              |
| 1:0:5:PHE:HB3      | 1:0:59:ILE:HD12    | 1.91                     | 0.52              |
| 7:6:17:DC:H42      | 8:7:35:G:H1        | 1.58                     | 0.52              |
| 9:9:43:LYS:O       | 9:9:47:GLU:OE1     | 2.28                     | 0.52              |
| 9:9:88:HIS:O       | 9:9:89:PRO:C       | 2.51                     | 0.52              |
| 14:AE:795:TYR:OH   | 14:AE:1326:GLN:NE2 | 2.42                     | 0.52              |
| 16:C:38:LYS:HE2    | 16:C:38:LYS:CA     | 2.37                     | 0.52              |
| 17:D:512:U:P       | 23:J:44:ARG:NH1    | 2.83                     | 0.52              |
| 17:D:842:U:H3'     | 17:D:843:U:C5'     | 2.39                     | 0.52              |
| 17:D:936:C:C2      | 17:D:937:A:C8      | 2.98                     | 0.52              |
| 17:D:1086:U:C2     | 17:D:1087:G:C8     | 2.97                     | 0.52              |
| 17:D:1371:G:O3'    | 28:O:71:GLY:HA3    | 2.10                     | 0.52              |
| 20:G:17:GLY:HA3    | 20:G:41:ILE:HD11   | 1.92                     | 0.52              |
| 27:N:66:PHE:CD2    | 27:N:67:GLN:OE1    | 2.62                     | 0.52              |
| 28:O:9:THR:HB      | 28:O:85:ARG:NH1    | 2.25                     | 0.52              |
| 30:Q:52:PHE:CZ     | 30:Q:65:VAL:HG21   | 2.45                     | 0.52              |
| 38:Y:126:ARG:NH1   | 40:a:1083:U:P      | 2.83                     | 0.52              |
| 40:a:632:A:H2'     | 40:a:633:A:C8      | 2.44                     | 0.52              |
| 40:a:2308:G:C6     | 53:n:77:PHE:CZ     | 2.97                     | 0.52              |
| 53:n:71:ARG:C      | 53:n:81:GLN:HE22   | 2.17                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 56:q:9:LYS:HZ3      | 56:q:11:CYS:C       | 2.18                     | 0.52              |
| 58:s:31:GLU:HG2     | 58:s:142:ILE:HG12   | 1.92                     | 0.52              |
| 59:t:20:MET:CB      | 59:t:44:LYS:HZ3     | 2.19                     | 0.52              |
| 59:t:99:ILE:HD13    | 59:t:118:LEU:CB     | 2.39                     | 0.52              |
| 60:u:14:LYS:HE2     | 60:u:14:LYS:HA      | 1.91                     | 0.52              |
| 61:v:112:LEU:HA     | 61:v:115:GLU:OE1    | 2.10                     | 0.52              |
| 4:3:6:ARG:HG3       | 40:a:84:A:H3'       | 1.91                     | 0.52              |
| 8:7:20:U:H5''       | 8:7:21:U:H5'        | 1.91                     | 0.52              |
| 9:9:51:TYR:HB2      | 9:9:88:HIS:HB2      | 1.90                     | 0.52              |
| 9:9:136:ILE:HG13    | 9:9:136:ILE:O       | 2.09                     | 0.52              |
| 11:AA:1117:LEU:HD12 | 11:AA:1195:ILE:HG12 | 1.90                     | 0.52              |
| 12:AB:141:LEU:O     | 12:AB:150:ILE:C     | 2.53                     | 0.52              |
| 14:AE:959:LYS:HB3   | 14:AE:983:LYS:HB2   | 1.92                     | 0.52              |
| 10:B:48:C:O2'       | 10:B:49:G:OP2       | 2.27                     | 0.52              |
| 17:D:452:A:H2'      | 17:D:453:G:O4'      | 2.10                     | 0.52              |
| 17:D:978:A:C4       | 17:D:1319:A:C2      | 2.98                     | 0.52              |
| 21:H:36:VAL:O       | 21:H:48:ILE:HB      | 2.10                     | 0.52              |
| 28:O:88:MET:HE1     | 28:O:95:ARG:HG3     | 1.91                     | 0.52              |
| 28:O:118:LEU:HD23   | 28:O:124:ARG:HA     | 1.91                     | 0.52              |
| 31:R:24:LEU:C       | 31:R:25:GLU:OE1     | 2.52                     | 0.52              |
| 33:T:64:ARG:NH2     | 33:T:89:ARG:HH22    | 2.07                     | 0.52              |
| 36:W:17:LYS:HB3     | 36:W:21:LYS:HZ3     | 1.74                     | 0.52              |
| 37:X:22:ILE:HB      | 37:X:25:VAL:CG1     | 2.39                     | 0.52              |
| 40:a:150:U:H2'      | 40:a:151:C:C6       | 2.44                     | 0.52              |
| 40:a:743:A:O2'      | 40:a:1659:G:OP1     | 2.25                     | 0.52              |
| 40:a:1243:C:H1'     | 60:u:4:ASN:O        | 2.09                     | 0.52              |
| 40:a:1394:U:H4'     | 40:a:1603:A:H4'     | 1.92                     | 0.52              |
| 40:a:2287:A:C8      | 40:a:2289:G:C8      | 2.96                     | 0.52              |
| 51:l:6:LYS:CE       | 51:l:119:ILE:HG23   | 2.40                     | 0.52              |
| 55:p:9:VAL:HG22     | 55:p:69:ARG:NH1     | 2.24                     | 0.52              |
| 59:t:71:ARG:NH2     | 59:t:123:LEU:O      | 2.42                     | 0.52              |
| 61:v:114:ARG:C      | 61:v:118:LYS:HZ3    | 2.18                     | 0.52              |
| 6:5:17:DC:H5''      | 6:5:17:DC:H6        | 1.75                     | 0.52              |
| 7:6:23:DC:H5'       | 14:AE:259:ARG:NH1   | 2.11                     | 0.52              |
| 9:9:59:LEU:HB2      | 9:9:62:ARG:HG3      | 1.91                     | 0.52              |
| 11:AA:125:GLY:HA2   | 11:AA:499:SER:HB2   | 1.92                     | 0.52              |
| 11:AA:855:PRO:HD2   | 11:AA:887:VAL:HG11  | 1.91                     | 0.52              |
| 12:AB:51:PHE:CZ     | 14:AE:288:PRO:CG    | 2.89                     | 0.52              |
| 10:B:31:G:H2'       | 10:B:32:C:O4'       | 2.10                     | 0.52              |
| 17:D:122:G:C5       | 17:D:123:U:C5       | 2.98                     | 0.52              |
| 17:D:925:G:C2       | 17:D:927:G:C8       | 2.98                     | 0.52              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 17:D:1158:C:O2'    | 20:G:132:LYS:HE2    | 2.09                     | 0.52              |
| 18:E:75:HIS:CE1    | 18:E:79:LEU:CD1     | 2.93                     | 0.52              |
| 21:H:335:ILE:HG12  | 21:H:342:ILE:HD12   | 1.92                     | 0.52              |
| 22:I:178:LEU:HD23  | 22:I:178:LEU:C      | 2.35                     | 0.52              |
| 32:S:87:ALA:N      | 32:S:90:ARG:NH1     | 2.58                     | 0.52              |
| 40:a:65:U:H2'      | 40:a:66:C:H6        | 1.75                     | 0.52              |
| 40:a:139:U:OP2     | 40:a:140:C:N4       | 2.43                     | 0.52              |
| 40:a:888:C:C4      | 40:a:889:C:C4       | 2.97                     | 0.52              |
| 40:a:963:U:C2      | 40:a:964:C:C5       | 2.97                     | 0.52              |
| 40:a:1095:A:H2'    | 40:a:1096:A:C8      | 2.45                     | 0.52              |
| 40:a:1707:G:C8     | 40:a:1756:G:C5      | 2.98                     | 0.52              |
| 40:a:1996:C:H4'    | 49:j:128:ARG:HH12   | 1.75                     | 0.52              |
| 47:h:76:ALA:HB1    | 47:h:94:VAL:CG1     | 2.39                     | 0.52              |
| 50:k:19:HIS:CE1    | 50:k:41:PRO:HD3     | 2.45                     | 0.52              |
| 57:r:29:PHE:CE2    | 57:r:35:LYS:HE3     | 2.45                     | 0.52              |
| 61:v:105:MET:HE2   | 61:v:108:VAL:CG2    | 2.40                     | 0.52              |
| 4:3:66:GLN:OE1     | 4:3:69:ASN:ND2      | 2.44                     | 0.51              |
| 9:9:43:LYS:HZ2     | 9:9:101:LYS:HE2     | 1.74                     | 0.51              |
| 10:A:6:G:C4        | 10:A:7:G:C8         | 2.98                     | 0.51              |
| 11:AA:628:HIS:HB3  | 11:AA:647:ARG:HH21  | 1.73                     | 0.51              |
| 12:AB:148:LYS:HE3  | 29:P:102:LEU:HB3    | 1.88                     | 0.51              |
| 14:AE:901:ARG:HH21 | 14:AE:906:GLY:HA2   | 1.73                     | 0.51              |
| 28:O:123:ARG:O     | 28:O:123:ARG:CG     | 2.57                     | 0.51              |
| 29:P:73:LEU:HD21   | 29:P:75:ASP:OD2     | 2.10                     | 0.51              |
| 31:R:62:GLU:OE2    | 31:R:62:GLU:HA      | 2.11                     | 0.51              |
| 33:T:24:SER:O      | 33:T:28:GLN:HG2     | 2.09                     | 0.51              |
| 37:X:68:ASP:O      | 37:X:71:ARG:HG3     | 2.09                     | 0.51              |
| 40:a:628:G:C5      | 40:a:636:G:N2       | 2.79                     | 0.51              |
| 40:a:658:U:O2'     | 51:l:97:ASN:OD1     | 2.28                     | 0.51              |
| 40:a:833:A:H2'     | 40:a:834:G:C8       | 2.44                     | 0.51              |
| 40:a:1453:A:C8     | 62:w:73:ASN:OD1     | 2.64                     | 0.51              |
| 40:a:1681:G:H2'    | 40:a:1757:A:N1      | 2.25                     | 0.51              |
| 40:a:2086:U:H2'    | 40:a:2087:G:C8      | 2.46                     | 0.51              |
| 43:d:15:A:O4'      | 43:d:109:A:C8       | 2.63                     | 0.51              |
| 53:n:136:ILE:HD12  | 53:n:141:ILE:HG23   | 1.92                     | 0.51              |
| 62:w:24:MET:HA     | 62:w:24:MET:CE      | 2.33                     | 0.51              |
| 5:4:2:PHE:CE2      | 5:4:55:GLU:HG2      | 2.45                     | 0.51              |
| 8:7:2:U:H2'        | 8:7:3:G:C8          | 2.45                     | 0.51              |
| 9:9:87:GLU:OE2     | 9:9:95:LEU:HG       | 2.09                     | 0.51              |
| 11:AA:974:ARG:HD2  | 11:AA:1014:LEU:HD21 | 1.92                     | 0.51              |
| 12:AB:141:LEU:HA   | 12:AB:152:HIS:HA    | 1.92                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:B:48:C:C5      | 10:B:59:A:C8       | 2.98                     | 0.51              |
| 16:C:60:LYS:CE    | 17:D:735:C:C4'     | 2.88                     | 0.51              |
| 17:D:1176:A:H2'   | 17:D:1177:G:C8     | 2.45                     | 0.51              |
| 20:G:165:ASP:O    | 20:G:169:GLU:OE1   | 2.28                     | 0.51              |
| 24:K:134:ILE:HG23 | 24:K:135:ASN:N     | 2.24                     | 0.51              |
| 25:L:33:GLU:HG3   | 25:L:33:GLU:O      | 2.10                     | 0.51              |
| 25:L:88:MET:HE2   | 25:L:90:MET:HE3    | 1.91                     | 0.51              |
| 28:O:7:TYR:H      | 28:O:89:GLU:CD     | 2.19                     | 0.51              |
| 35:V:62:ARG:CA    | 35:V:73:TRP:CZ3    | 2.93                     | 0.51              |
| 38:Y:55:PRO:C     | 38:Y:71:LYS:HE2    | 2.36                     | 0.51              |
| 39:Z:26:MET:HA    | 39:Z:30:PHE:CD1    | 2.46                     | 0.51              |
| 46:g:47:LYS:HE2   | 53:n:115:ARG:NE    | 2.25                     | 0.51              |
| 47:h:18:LYS:HE3   | 47:h:20:VAL:CG2    | 2.41                     | 0.51              |
| 49:j:122:VAL:HG21 | 49:j:141:ARG:HG3   | 1.92                     | 0.51              |
| 53:n:30:ARG:HB2   | 53:n:30:ARG:NH2    | 2.25                     | 0.51              |
| 61:v:45:GLN:HE21  | 61:v:124:LEU:HA    | 1.75                     | 0.51              |
| 61:v:115:GLU:HA   | 61:v:118:LYS:NZ    | 2.25                     | 0.51              |
| 1:0:17:GLY:HA2    | 1:0:97:LYS:HE2     | 1.92                     | 0.51              |
| 10:A:23:C:H2'     | 10:A:24:U:C6       | 2.45                     | 0.51              |
| 12:AB:141:LEU:HA  | 12:AB:152:HIS:CA   | 2.39                     | 0.51              |
| 16:C:70:TYR:CE2   | 25:L:49:TYR:CZ     | 2.98                     | 0.51              |
| 16:C:71:THR:H     | 16:C:74:HIS:HE1    | 1.58                     | 0.51              |
| 17:D:718:A:H5'    | 30:Q:119:ASN:HD22  | 1.76                     | 0.51              |
| 17:D:868:C:H2'    | 17:D:869:G:O4'     | 2.11                     | 0.51              |
| 21:H:321:VAL:HG13 | 21:H:322:VAL:HG23  | 1.91                     | 0.51              |
| 22:I:23:PHE:HD2   | 29:P:97:ASP:HB2    | 1.74                     | 0.51              |
| 22:I:68:ILE:HG13  | 22:I:101:ILE:HD11  | 1.93                     | 0.51              |
| 37:X:13:LYS:HE3   | 37:X:17:ILE:HG21   | 1.91                     | 0.51              |
| 40:a:626:A:N3     | 60:u:78:ARG:CZ     | 2.74                     | 0.51              |
| 40:a:1198:U:C2    | 40:a:1199:U:C5     | 2.98                     | 0.51              |
| 40:a:2812:G:H2'   | 40:a:2813:A:C8     | 2.45                     | 0.51              |
| 49:j:68:PHE:CD2   | 49:j:75:ALA:HA     | 2.46                     | 0.51              |
| 58:s:98:GLU:O     | 58:s:99:ARG:C      | 2.53                     | 0.51              |
| 61:v:53:MET:HE3   | 61:v:120:ALA:CB    | 2.40                     | 0.51              |
| 64:y:9:GLU:CG     | 64:y:55:LEU:HB2    | 2.40                     | 0.51              |
| 1:0:1:MET:O       | 1:0:15:SER:OG      | 2.19                     | 0.51              |
| 2:1:25:ARG:NH1    | 40:a:519:U:O3'     | 2.43                     | 0.51              |
| 3:2:11:LEU:HD12   | 3:2:11:LEU:N       | 2.26                     | 0.51              |
| 11:AA:714:VAL:HB  | 11:AA:787:PRO:HD2  | 1.92                     | 0.51              |
| 12:AB:89:PRO:HG2  | 14:AE:290:ILE:HG22 | 1.91                     | 0.51              |
| 17:D:500:G:H2'    | 17:D:501:C:C6      | 2.45                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:D:679:C:H2'     | 17:D:680:C:H6      | 1.74                     | 0.51              |
| 20:G:16:PHE:HB3    | 21:H:43:LYS:HA     | 1.93                     | 0.51              |
| 36:W:45:ILE:HA     | 36:W:62:VAL:HG11   | 1.92                     | 0.51              |
| 40:a:414:C:H2'     | 40:a:415:A:H8      | 1.75                     | 0.51              |
| 40:a:2329:U:H2'    | 40:a:2330:G:C8     | 2.45                     | 0.51              |
| 40:a:2420:C:H5''   | 50:k:8:LYS:HE2     | 1.92                     | 0.51              |
| 40:a:2588:G:O6     | 40:a:2607:G:C6     | 2.64                     | 0.51              |
| 49:j:152:PRO:CG    | 49:j:156:PHE:CZ    | 2.91                     | 0.51              |
| 50:k:9:ILE:CG2     | 50:k:27:LYS:HZ1    | 2.23                     | 0.51              |
| 50:k:21:TYR:CE2    | 50:k:49:TYR:CE2    | 2.99                     | 0.51              |
| 54:o:19:LYS:HE2    | 54:o:19:LYS:HA     | 1.91                     | 0.51              |
| 59:t:103:VAL:HG21  | 59:t:107:LEU:CD2   | 2.41                     | 0.51              |
| 62:w:82:GLU:OE1    | 62:w:82:GLU:N      | 2.44                     | 0.51              |
| 65:z:65:ILE:HB     | 65:z:76:TYR:HE1    | 1.75                     | 0.51              |
| 3:2:3:ARG:NH2      | 3:2:4:GLU:HB2      | 2.26                     | 0.51              |
| 5:4:48:MET:CE      | 5:4:86:LEU:HG      | 2.40                     | 0.51              |
| 12:AB:10:LYS:HB2   | 12:AB:73:ARG:HB3   | 1.90                     | 0.51              |
| 12:AB:136:GLU:HA   | 12:AB:159:PHE:CZ   | 2.46                     | 0.51              |
| 14:AE:510:LEU:HD22 | 14:AE:601:ILE:HD12 | 1.91                     | 0.51              |
| 10:B:56:C:H2'      | 10:B:57:A:H5''     | 1.93                     | 0.51              |
| 17:D:58:C:O2       | 17:D:58:C:H2'      | 2.09                     | 0.51              |
| 17:D:107:G:C6      | 18:E:10:ARG:NH2    | 2.79                     | 0.51              |
| 17:D:564:C:H5'     | 35:V:34:TYR:CE1    | 2.46                     | 0.51              |
| 22:I:108:LYS:N     | 22:I:108:LYS:HD2   | 2.26                     | 0.51              |
| 25:L:4:TYR:OH      | 25:L:68:GLN:HG2    | 2.11                     | 0.51              |
| 25:L:45:ARG:HA     | 25:L:45:ARG:NE     | 2.26                     | 0.51              |
| 25:L:67:PRO:O      | 25:L:70:VAL:HG22   | 2.11                     | 0.51              |
| 29:P:22:THR:O      | 29:P:25:ILE:HG22   | 2.10                     | 0.51              |
| 29:P:24:GLU:O      | 29:P:28:THR:HG23   | 2.10                     | 0.51              |
| 40:a:607:U:C5      | 40:a:620:G:C5      | 2.97                     | 0.51              |
| 40:a:703:U:H2'     | 40:a:704:G:O4'     | 2.10                     | 0.51              |
| 40:a:872:U:H2'     | 40:a:873:C:H6      | 1.75                     | 0.51              |
| 40:a:960:A:H61     | 61:v:82:MET:CE     | 2.23                     | 0.51              |
| 40:a:1138:G:C2     | 58:s:108:MET:HE2   | 2.45                     | 0.51              |
| 40:a:2252:G:H2'    | 40:a:2253:G:H8     | 1.76                     | 0.51              |
| 40:a:2387:U:C4'    | 41:b:41:ARG:HH12   | 2.24                     | 0.51              |
| 40:a:2428:G:H21    | 60:u:60:ARG:CZ     | 2.23                     | 0.51              |
| 40:a:2473:U:C4     | 40:a:2474:U:C5     | 2.97                     | 0.51              |
| 40:a:2682:A:C2     | 49:j:23:PRO:HB3    | 2.46                     | 0.51              |
| 53:n:8:TYR:HE2     | 53:n:30:ARG:HE     | 1.59                     | 0.51              |
| 60:u:90:VAL:CG1    | 60:u:95:LEU:HD21   | 2.33                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 65:z:74:ILE:HG13  | 65:z:78:LYS:CE    | 2.40                     | 0.51              |
| 4:3:85:PHE:CE1    | 4:3:94:ARG:HG2    | 2.46                     | 0.51              |
| 5:4:2:PHE:CE1     | 5:4:56:PHE:CE1    | 2.99                     | 0.51              |
| 9:9:94:ARG:HB2    | 9:9:97:LYS:CE     | 2.36                     | 0.51              |
| 10:A:48:C:C5      | 10:A:59:A:C8      | 2.98                     | 0.51              |
| 10:B:6:G:C4       | 10:B:7:G:C8       | 2.98                     | 0.51              |
| 17:D:107:G:C5     | 18:E:10:ARG:NH2   | 2.79                     | 0.51              |
| 17:D:512:U:P      | 23:J:44:ARG:HH12  | 2.34                     | 0.51              |
| 17:D:934:C:C4     | 17:D:1345:U:C5    | 2.98                     | 0.51              |
| 19:F:36:GLU:OE2   | 19:F:36:GLU:HA    | 2.11                     | 0.51              |
| 20:G:26:LYS:HD2   | 20:G:193:PRO:CG   | 2.40                     | 0.51              |
| 21:H:32:ASP:OD1   | 21:H:35:VAL:CG2   | 2.57                     | 0.51              |
| 21:H:279:LYS:HA   | 21:H:331:MET:CB   | 2.41                     | 0.51              |
| 31:R:3:THR:O      | 31:R:6:GLN:N      | 2.44                     | 0.51              |
| 32:S:10:GLU:OE2   | 32:S:63:ARG:HD2   | 2.11                     | 0.51              |
| 40:a:910:A:C8     | 61:v:12:MET:CE    | 2.94                     | 0.51              |
| 40:a:1314:C:C2    | 40:a:1315:C:C5    | 2.98                     | 0.51              |
| 40:a:1666:G:P     | 59:t:66:LYS:HD3   | 2.50                     | 0.51              |
| 40:a:2093:G:OP2   | 57:r:22:LYS:HG2   | 2.11                     | 0.51              |
| 40:a:2698:U:H2'   | 40:a:2699:C:C6    | 2.46                     | 0.51              |
| 60:u:58:TYR:CE2   | 60:u:59:ARG:HG2   | 2.44                     | 0.51              |
| 60:u:122:VAL:HG13 | 60:u:125:LEU:CD1  | 2.34                     | 0.51              |
| 65:z:65:ILE:HB    | 65:z:76:TYR:CE1   | 2.45                     | 0.51              |
| 1:0:37:GLU:O      | 1:0:37:GLU:HG3    | 2.11                     | 0.51              |
| 14:AE:71:LEU:HD22 | 14:AE:90:VAL:HG21 | 1.93                     | 0.51              |
| 17:D:501:C:H2'    | 17:D:502:A:H8     | 1.75                     | 0.51              |
| 17:D:1226:C:C2'   | 37:X:102:THR:OG1  | 2.58                     | 0.51              |
| 24:K:36:LEU:HD13  | 24:K:134:ILE:CD1  | 2.40                     | 0.51              |
| 29:P:7:ARG:HD3    | 29:P:75:ASP:OD1   | 2.10                     | 0.51              |
| 39:Z:15:SER:O     | 39:Z:19:VAL:HG23  | 2.11                     | 0.51              |
| 40:a:413:C:C2     | 40:a:414:C:C5     | 2.99                     | 0.51              |
| 40:a:1154:G:OP2   | 65:z:58:ARG:CZ    | 2.58                     | 0.51              |
| 40:a:1668:A:O2'   | 40:a:1674:G:N7    | 2.32                     | 0.51              |
| 40:a:1853:A:H2'   | 40:a:1854:A:C8    | 2.46                     | 0.51              |
| 40:a:2266:A:H4'   | 40:a:2267:A:N3    | 2.26                     | 0.51              |
| 43:d:42:C:P       | 53:n:64:LYS:NZ    | 2.83                     | 0.51              |
| 48:i:30:VAL:HG22  | 48:i:37:LYS:CD    | 2.41                     | 0.51              |
| 49:j:154:LYS:HE3  | 49:j:156:PHE:CE1  | 2.46                     | 0.51              |
| 53:n:15:LYS:O     | 53:n:18:THR:N     | 2.43                     | 0.51              |
| 55:p:149:ARG:CZ   | 55:p:154:PRO:HD3  | 2.40                     | 0.51              |
| 63:x:53:THR:HG23  | 63:x:74:VAL:HG21  | 1.92                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:5:9:DG:P         | 11:AA:473:ARG:HG3 | 2.51                     | 0.51              |
| 8:7:13:U:H5''      | 8:7:13:U:C6       | 2.45                     | 0.51              |
| 10:A:56:C:C5       | 40:a:2168:G:C6    | 2.98                     | 0.51              |
| 14:AE:77:ARG:HB3   | 14:AE:80:HIS:HB2  | 1.93                     | 0.51              |
| 17:D:49:U:C2       | 17:D:361:G:N2     | 2.79                     | 0.51              |
| 17:D:739:C:HO2'    | 33:T:42:HIS:CE1   | 2.25                     | 0.51              |
| 17:D:754:C:OP1     | 33:T:72:ARG:NH1   | 2.44                     | 0.51              |
| 20:G:9:MET:HE1     | 20:G:47:VAL:CG2   | 2.40                     | 0.51              |
| 20:G:26:LYS:HE3    | 20:G:194:ASP:OD1  | 2.10                     | 0.51              |
| 20:G:90:PHE:CD2    | 20:G:154:MET:CE   | 2.94                     | 0.51              |
| 21:H:163:ARG:CA    | 21:H:298:GLU:HG3  | 2.41                     | 0.51              |
| 24:K:156:LYS:NZ    | 27:N:71:VAL:O     | 2.42                     | 0.51              |
| 28:O:30:ILE:HD13   | 28:O:39:PHE:HE2   | 1.75                     | 0.51              |
| 31:R:109:ASP:C     | 31:R:111:LYS:HZ3  | 2.18                     | 0.51              |
| 31:R:110:ARG:HE    | 31:R:117:TYR:HD2  | 1.57                     | 0.51              |
| 37:X:31:LYS:HG3    | 37:X:32:ALA:N     | 2.25                     | 0.51              |
| 38:Y:41:PHE:O      | 38:Y:45:THR:OG1   | 2.22                     | 0.51              |
| 40:a:1656:C:OP1    | 49:j:141:ARG:HD3  | 2.10                     | 0.51              |
| 40:a:1791:A:C2     | 40:a:1829:A:C4'   | 2.94                     | 0.51              |
| 40:a:2006:C:C2     | 40:a:2007:U:C5    | 2.99                     | 0.51              |
| 40:a:2311:A:C5     | 53:n:77:PHE:CD2   | 2.98                     | 0.51              |
| 47:h:130:LEU:HD21  | 47:h:192:LEU:HD21 | 1.93                     | 0.51              |
| 58:s:35:ARG:HA     | 58:s:40:HIS:CE1   | 2.46                     | 0.51              |
| 62:w:24:MET:HE3    | 62:w:24:MET:CA    | 2.34                     | 0.51              |
| 65:z:53:ARG:HG3    | 65:z:57:PHE:HE2   | 1.75                     | 0.51              |
| 5:4:51:GLN:OE1     | 5:4:57:TYR:OH     | 2.27                     | 0.51              |
| 12:AB:78:PHE:CG    | 12:AB:85:PRO:HB3  | 2.46                     | 0.51              |
| 12:AB:81:PHE:CB    | 14:AE:141:PHE:O   | 2.58                     | 0.51              |
| 14:AE:1179:PRO:HB2 | 14:AE:1182:GLY:H  | 1.75                     | 0.51              |
| 29:P:24:GLU:CA     | 29:P:27:GLU:OE1   | 2.59                     | 0.51              |
| 30:Q:23:ILE:N      | 30:Q:87:LYS:HZ1   | 2.09                     | 0.51              |
| 31:R:54:ARG:HH11   | 31:R:62:GLU:HG3   | 1.76                     | 0.51              |
| 33:T:3:LEU:HD23    | 33:T:3:LEU:C      | 2.36                     | 0.51              |
| 38:Y:126:ARG:HD2   | 38:Y:127:SER:N    | 2.26                     | 0.51              |
| 40:a:372:G:C8      | 42:c:61:LYS:HD2   | 2.46                     | 0.51              |
| 40:a:532:A:H4'     | 40:a:533:G:C8     | 2.46                     | 0.51              |
| 40:a:993:G:C6      | 40:a:1162:G:C6    | 2.99                     | 0.51              |
| 40:a:1346:G:C6     | 40:a:1601:G:C6    | 2.98                     | 0.51              |
| 40:a:1824:G:O2'    | 47:h:252:THR:HG21 | 2.11                     | 0.51              |
| 40:a:1999:C:O3'    | 40:a:2722:G:N2    | 2.44                     | 0.51              |
| 40:a:2133:G:O2'    | 40:a:2157:G:N2    | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:a:2298:A:O3'   | 53:n:72:LYS:HE2   | 2.11                     | 0.51              |
| 40:a:2814:A:H2'   | 40:a:2815:C:H6    | 1.75                     | 0.51              |
| 45:f:41:THR:N     | 45:f:45:ARG:HH22  | 2.09                     | 0.51              |
| 46:g:7:PRO:HD2    | 53:n:62:GLY:O     | 2.11                     | 0.51              |
| 47:h:124:ILE:O    | 47:h:125:LYS:HD3  | 2.10                     | 0.51              |
| 55:p:127:THR:HG22 | 55:p:128:GLN:N    | 2.26                     | 0.51              |
| 61:v:31:PHE:O     | 61:v:104:GLU:CD   | 2.54                     | 0.51              |
| 63:x:4:LYS:N      | 63:x:4:LYS:HD3    | 2.26                     | 0.51              |
| 65:z:82:GLY:HA3   | 65:z:117:LEU:CD1  | 2.41                     | 0.51              |
| 5:4:48:MET:HE2    | 5:4:86:LEU:HG     | 1.93                     | 0.51              |
| 8:7:3:G:C4'       | 17:D:1500:A:N6    | 2.74                     | 0.51              |
| 8:7:28:U:O2       | 8:7:28:U:H2'      | 2.10                     | 0.51              |
| 10:A:31:G:H2'     | 10:A:32:C:O4'     | 2.10                     | 0.51              |
| 10:A:33:U:H5''    | 26:M:84:THR:HG21  | 1.93                     | 0.51              |
| 17:D:335:C:C2     | 17:D:336:A:C8     | 2.99                     | 0.51              |
| 17:D:612:C:C2     | 17:D:613:C:C5     | 2.99                     | 0.51              |
| 17:D:678:U:H2'    | 17:D:679:C:H6     | 1.76                     | 0.51              |
| 17:D:767:A:H2'    | 17:D:768:A:O4'    | 2.11                     | 0.51              |
| 17:D:1106:G:O3'   | 22:I:172:ARG:HG3  | 2.11                     | 0.51              |
| 20:G:35:ARG:HB3   | 21:H:14:LYS:NZ    | 2.26                     | 0.51              |
| 21:H:273:ARG:NH1  | 21:H:297:GLU:HB2  | 2.25                     | 0.51              |
| 29:P:15:HIS:HB3   | 29:P:70:HIS:CE1   | 2.46                     | 0.51              |
| 34:U:39:PHE:CD1   | 34:U:50:THR:HG22  | 2.45                     | 0.51              |
| 37:X:71:ARG:HH12  | 46:g:52:ALA:HB3   | 1.75                     | 0.51              |
| 40:a:271:G:H4'    | 40:a:272:A:OP1    | 2.10                     | 0.51              |
| 40:a:413:C:H2'    | 40:a:414:C:C6     | 2.46                     | 0.51              |
| 40:a:580:U:H2'    | 40:a:581:C:C6     | 2.46                     | 0.51              |
| 40:a:1589:U:O2'   | 40:a:1590:A:O5'   | 2.28                     | 0.51              |
| 40:a:1598:A:C5    | 40:a:1599:U:C5    | 2.99                     | 0.51              |
| 40:a:1790:C:C3'   | 40:a:1791:A:C8    | 2.94                     | 0.51              |
| 41:b:55:ARG:HA    | 41:b:55:ARG:CZ    | 2.41                     | 0.51              |
| 44:e:20:ASN:HA    | 44:e:23:ARG:HE    | 1.76                     | 0.51              |
| 45:f:4:THR:CB     | 45:f:37:GLU:OE2   | 2.58                     | 0.51              |
| 49:j:184:ARG:HH12 | 64:y:7:GLN:NE2    | 2.09                     | 0.51              |
| 55:p:162:VAL:O    | 55:p:162:VAL:HG12 | 2.11                     | 0.51              |
| 57:r:71:LYS:HZ2   | 57:r:72:ILE:HA    | 1.75                     | 0.51              |
| 58:s:15:TRP:CZ3   | 58:s:135:GLN:CA   | 2.93                     | 0.51              |
| 58:s:84:ILE:HG23  | 58:s:84:ILE:O     | 2.11                     | 0.51              |
| 60:u:58:TYR:CD2   | 60:u:59:ARG:HG2   | 2.46                     | 0.51              |
| 3:2:19:LYS:NZ     | 40:a:1340:U:OP1   | 2.34                     | 0.50              |
| 8:7:12:U:H5''     | 24:K:56:VAL:HG21  | 1.93                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:9:106:PHE:CG     | 9:9:106:PHE:O     | 2.63                     | 0.50              |
| 10:A:23:C:H2'      | 10:A:24:U:H6      | 1.77                     | 0.50              |
| 12:AB:134:ASP:OD1  | 12:AB:135:GLY:N   | 2.37                     | 0.50              |
| 12:AB:147:ASN:CA   | 29:P:100:ILE:CG2  | 2.86                     | 0.50              |
| 13:AC:140:ILE:HD12 | 13:AC:142:MET:HE3 | 1.91                     | 0.50              |
| 14:AE:79:LYS:CA    | 14:AE:81:ARG:HH12 | 1.96                     | 0.50              |
| 10:B:23:C:H2'      | 10:B:24:U:C6      | 2.46                     | 0.50              |
| 16:C:51:TYR:O      | 16:C:54:GLN:HG3   | 2.11                     | 0.50              |
| 17:D:276:G:C5'     | 35:V:17:MET:CE    | 2.89                     | 0.50              |
| 17:D:564:C:H5'     | 35:V:34:TYR:HE1   | 1.75                     | 0.50              |
| 17:D:580:C:H2'     | 17:D:581:G:O4'    | 2.12                     | 0.50              |
| 17:D:864:A:H2'     | 17:D:865:A:C8     | 2.46                     | 0.50              |
| 17:D:975:A:H8      | 17:D:1357:A:HO2'  | 1.58                     | 0.50              |
| 20:G:23:TRP:CD1    | 20:G:39:HIS:CE1   | 2.97                     | 0.50              |
| 26:M:66:LEU:CD1    | 26:M:101:MET:CE   | 2.84                     | 0.50              |
| 40:a:1318:U:C2     | 40:a:1319:C:C5    | 2.99                     | 0.50              |
| 40:a:2230:G:C5'    | 42:c:30:LEU:HD23  | 2.41                     | 0.50              |
| 40:a:2230:G:H5'    | 42:c:30:LEU:HD23  | 1.93                     | 0.50              |
| 40:a:2466:C:N3     | 40:a:2467:C:C5    | 2.79                     | 0.50              |
| 48:i:26:THR:HG23   | 48:i:27:SER:N     | 2.25                     | 0.50              |
| 51:l:168:ASP:HB3   | 51:l:183:PHE:HE2  | 1.75                     | 0.50              |
| 59:t:17:ARG:NH2    | 59:t:47:ILE:HG23  | 2.25                     | 0.50              |
| 59:t:34:GLY:N      | 59:t:37:ASP:OD2   | 2.40                     | 0.50              |
| 9:9:55:VAL:CG1     | 9:9:56:ARG:N      | 2.74                     | 0.50              |
| 13:AD:15:ASP:OD1   | 13:AD:27:THR:OG1  | 2.29                     | 0.50              |
| 17:D:21:G:C2       | 17:D:22:G:C5      | 2.99                     | 0.50              |
| 30:Q:63:ALA:HB1    | 30:Q:96:THR:CG2   | 2.41                     | 0.50              |
| 33:T:3:LEU:HD12    | 33:T:35:GLN:OE1   | 2.10                     | 0.50              |
| 33:T:5:THR:HG23    | 33:T:6:GLU:N      | 2.25                     | 0.50              |
| 36:W:41:PHE:O      | 36:W:44:MET:HG3   | 2.11                     | 0.50              |
| 40:a:560:C:O2      | 65:z:48:ARG:NH1   | 2.37                     | 0.50              |
| 40:a:2063:C:O2     | 40:a:2450:A:N1    | 2.44                     | 0.50              |
| 40:a:2305:U:H4'    | 53:n:133:ARG:NH2  | 2.25                     | 0.50              |
| 40:a:2387:U:H4'    | 41:b:41:ARG:HH12  | 1.76                     | 0.50              |
| 40:a:2636:C:O2'    | 49:j:45:TYR:OH    | 1.99                     | 0.50              |
| 42:c:71:LEU:HB3    | 42:c:76:GLU:CG    | 2.41                     | 0.50              |
| 51:l:155:GLU:HG2   | 51:l:156:ASN:N    | 2.27                     | 0.50              |
| 51:l:194:LYS:O     | 51:l:197:GLU:N    | 2.45                     | 0.50              |
| 60:u:55:MET:HE1    | 60:u:60:ARG:HA    | 1.94                     | 0.50              |
| 61:v:73:ILE:HD12   | 61:v:73:ILE:N     | 2.26                     | 0.50              |
| 5:4:50:MET:CA      | 5:4:56:PHE:CZ     | 2.94                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:5:9:DG:OP2       | 11:AA:470:ARG:O    | 2.28                     | 0.50              |
| 9:9:58:THR:HG21    | 9:9:81:LEU:CD2     | 2.31                     | 0.50              |
| 9:9:78:GLY:H       | 9:9:79:PRO:HD2     | 1.75                     | 0.50              |
| 10:A:19:G:N2       | 40:a:2112:G:O4'    | 2.44                     | 0.50              |
| 12:AB:27:ASN:OD1   | 12:AB:58:GLU:HB2   | 2.11                     | 0.50              |
| 14:AE:157:GLN:HE22 | 14:AE:188:LEU:HD22 | 1.76                     | 0.50              |
| 17:D:160:A:H2'     | 17:D:161:A:O4'     | 2.12                     | 0.50              |
| 17:D:728:A:H2'     | 17:D:729:A:C8      | 2.46                     | 0.50              |
| 22:I:132:ARG:HG3   | 22:I:135:LYS:HE3   | 1.92                     | 0.50              |
| 22:I:142:MET:HE3   | 22:I:170:GLU:C     | 2.36                     | 0.50              |
| 24:K:111:MET:O     | 24:K:114:VAL:HG12  | 2.11                     | 0.50              |
| 26:M:35:LYS:HE3    | 26:M:38:THR:OG1    | 2.11                     | 0.50              |
| 29:P:66:GLU:CG     | 32:S:99:ALA:HB2    | 2.41                     | 0.50              |
| 30:Q:27:PHE:CE2    | 30:Q:89:PRO:HG2    | 2.46                     | 0.50              |
| 38:Y:126:ARG:CZ    | 40:a:1083:U:P      | 3.00                     | 0.50              |
| 40:a:299:A:N1      | 40:a:322:A:O2'     | 2.42                     | 0.50              |
| 40:a:1141:U:H5     | 58:s:68:LYS:HZ1    | 1.59                     | 0.50              |
| 40:a:1799:G:N2     | 47:h:154:LEU:HD23  | 2.26                     | 0.50              |
| 40:a:2391:G:P      | 54:o:32:ILE:HD12   | 2.50                     | 0.50              |
| 40:a:2848:G:O2'    | 40:a:2867:G:N2     | 2.36                     | 0.50              |
| 51:l:6:LYS:HZ2     | 51:l:119:ILE:HA    | 1.76                     | 0.50              |
| 52:m:25:LYS:C      | 52:m:29:GLN:HE22   | 2.20                     | 0.50              |
| 53:n:5:HIS:HD2     | 53:n:97:TRP:CZ2    | 2.29                     | 0.50              |
| 58:s:15:TRP:CD1    | 58:s:53:TYR:HB2    | 2.45                     | 0.50              |
| 61:v:105:MET:SD    | 61:v:113:ALA:HB1   | 2.52                     | 0.50              |
| 3:2:49:LYS:HE2     | 3:2:49:LYS:HA      | 1.93                     | 0.50              |
| 5:4:6:ALA:HB3      | 5:4:65:VAL:HG22    | 1.93                     | 0.50              |
| 6:5:16:DG:O6       | 11:AA:451:ARG:NH1  | 2.45                     | 0.50              |
| 9:9:47:GLU:O       | 9:9:49:GLY:N       | 2.43                     | 0.50              |
| 14:AE:67:ASP:C     | 14:AE:69:GLU:H     | 2.18                     | 0.50              |
| 17:D:653:U:O5'     | 27:N:56:LYS:HE2    | 2.12                     | 0.50              |
| 17:D:744:C:H2'     | 17:D:745:G:C8      | 2.47                     | 0.50              |
| 20:G:169:GLU:OE1   | 20:G:169:GLU:N     | 2.44                     | 0.50              |
| 21:H:48:ILE:HG22   | 21:H:49:PRO:O      | 2.10                     | 0.50              |
| 25:L:11:HIS:HB3    | 25:L:14:GLN:OE1    | 2.11                     | 0.50              |
| 27:N:106:THR:HB    | 27:N:121:LEU:CD1   | 2.41                     | 0.50              |
| 28:O:51:PRO:HA     | 28:O:103:PHE:HE2   | 1.76                     | 0.50              |
| 33:T:11:ILE:HD11   | 33:T:30:ALA:C      | 2.36                     | 0.50              |
| 35:V:15:ASP:OD1    | 35:V:55:ILE:HD11   | 2.11                     | 0.50              |
| 40:a:65:U:C2       | 40:a:66:C:C6       | 3.00                     | 0.50              |
| 40:a:995:C:O2      | 58:s:3:THR:OG1     | 2.17                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:a:2082:A:H2'    | 40:a:2083:G:O4'    | 2.12                     | 0.50              |
| 40:a:2259:U:C6     | 40:a:2427:C:C4     | 2.99                     | 0.50              |
| 40:a:2813:A:C4     | 40:a:2814:A:C8     | 2.99                     | 0.50              |
| 51:l:170:ARG:HH12  | 51:l:176:ASP:N     | 2.09                     | 0.50              |
| 54:o:31:HIS:O      | 54:o:32:ILE:C      | 2.54                     | 0.50              |
| 58:s:30:THR:HG23   | 58:s:31:GLU:N      | 2.26                     | 0.50              |
| 62:w:87:PHE:HZ     | 62:w:115:LEU:HG    | 1.77                     | 0.50              |
| 5:4:62:THR:OG1     | 5:4:71:LYS:HE3     | 2.11                     | 0.50              |
| 9:9:6:GLN:HA       | 9:9:9:GLN:HE22     | 1.74                     | 0.50              |
| 9:9:10:ALA:O       | 9:9:14:GLU:HG3     | 2.11                     | 0.50              |
| 9:9:30:SER:O       | 9:9:31:ARG:CZ      | 2.59                     | 0.50              |
| 9:9:52:MET:HG2     | 9:9:95:LEU:CD1     | 2.39                     | 0.50              |
| 12:AB:148:LYS:CE   | 29:P:102:LEU:HD23  | 2.41                     | 0.50              |
| 17:D:501:C:H2'     | 17:D:502:A:C8      | 2.46                     | 0.50              |
| 17:D:1073:U:O2'    | 20:G:105:LYS:HE3   | 2.11                     | 0.50              |
| 28:O:88:MET:SD     | 28:O:95:ARG:CZ     | 2.99                     | 0.50              |
| 36:W:49:ILE:HG23   | 36:W:49:ILE:O      | 2.12                     | 0.50              |
| 38:Y:37:PHE:HE1    | 38:Y:58:ILE:HD11   | 1.76                     | 0.50              |
| 38:Y:126:ARG:HD2   | 38:Y:126:ARG:C     | 2.36                     | 0.50              |
| 39:Z:18:ASP:HB3    | 39:Z:22:LEU:HD12   | 1.92                     | 0.50              |
| 40:a:125:A:C5      | 52:m:10:LEU:HD13   | 2.46                     | 0.50              |
| 40:a:851:C:C2      | 40:a:852:U:C5      | 3.00                     | 0.50              |
| 42:c:65:ASP:CG     | 42:c:66:THR:N      | 2.70                     | 0.50              |
| 46:g:58:ASP:CG     | 46:g:62:LYS:NZ     | 2.68                     | 0.50              |
| 49:j:55:LYS:NZ     | 49:j:59:ARG:C      | 2.70                     | 0.50              |
| 58:s:15:TRP:CH2    | 58:s:135:GLN:HG3   | 2.46                     | 0.50              |
| 58:s:74:TYR:N      | 58:s:74:TYR:HD2    | 2.10                     | 0.50              |
| 62:w:58:ASP:OD1    | 62:w:63:ARG:NH2    | 2.44                     | 0.50              |
| 3:2:12:ARG:HH21    | 44:e:29:ARG:CZ     | 2.25                     | 0.50              |
| 4:3:6:ARG:HG2      | 4:3:7:ARG:H        | 1.77                     | 0.50              |
| 10:A:68:C:C3'      | 10:A:69:C:H5''     | 2.42                     | 0.50              |
| 11:AA:146:VAL:HG21 | 11:AA:513:GLN:HE21 | 1.77                     | 0.50              |
| 11:AA:255:ILE:HB   | 11:AA:263:VAL:HB   | 1.92                     | 0.50              |
| 12:AB:130:PHE:CD2  | 12:AB:152:HIS:CE1  | 2.99                     | 0.50              |
| 12:AB:158:GLU:HB3  | 12:AB:162:LEU:CD2  | 2.42                     | 0.50              |
| 16:C:60:LYS:NZ     | 17:D:735:C:C5'     | 2.75                     | 0.50              |
| 16:C:60:LYS:HE3    | 17:D:735:C:C4'     | 2.42                     | 0.50              |
| 17:D:109:A:H2'     | 17:D:326:G:N2      | 2.27                     | 0.50              |
| 17:D:958:A:O4'     | 36:W:55:ARG:NH1    | 2.45                     | 0.50              |
| 18:E:54:MET:CE     | 18:E:75:HIS:HE1    | 2.24                     | 0.50              |
| 19:F:6:VAL:HG12    | 30:Q:108:THR:O     | 2.11                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 19:F:25:LYS:HE3    | 21:H:336:ASP:OD2  | 2.11                     | 0.50              |
| 20:G:109:GLN:C     | 20:G:113:ARG:HE   | 2.19                     | 0.50              |
| 20:G:187:VAL:HG13  | 20:G:191:SER:HB2  | 1.93                     | 0.50              |
| 37:X:65:VAL:HG23   | 37:X:66:GLU:OE1   | 2.12                     | 0.50              |
| 38:Y:57:VAL:HG23   | 38:Y:71:LYS:HD3   | 1.94                     | 0.50              |
| 40:a:756:A:H2'     | 40:a:757:G:O4'    | 2.11                     | 0.50              |
| 40:a:780:G:C2      | 40:a:782:A:C2     | 3.00                     | 0.50              |
| 40:a:813:U:H2'     | 40:a:814:C:C6     | 2.47                     | 0.50              |
| 40:a:1823:G:O2'    | 40:a:1824:G:H5'   | 2.12                     | 0.50              |
| 40:a:1956:U:C4     | 40:a:1957:C:C5    | 2.99                     | 0.50              |
| 40:a:2646:C:OP2    | 40:a:2732:G:O2'   | 2.25                     | 0.50              |
| 59:t:121:GLU:HG3   | 59:t:123:LEU:HD12 | 1.94                     | 0.50              |
| 62:w:12:ARG:NE     | 62:w:20:MET:HE1   | 2.26                     | 0.50              |
| 64:y:106:LYS:HD3   | 64:y:109:ARG:NH2  | 2.26                     | 0.50              |
| 12:AB:102:LYS:NZ   | 14:AE:285:LEU:HG  | 2.27                     | 0.50              |
| 12:AB:142:LEU:HD12 | 12:AB:150:ILE:O   | 2.11                     | 0.50              |
| 16:C:24:LYS:HB3    | 25:L:102:MET:HE1  | 1.93                     | 0.50              |
| 16:C:41:PRO:HD2    | 21:H:339:ARG:NE   | 2.26                     | 0.50              |
| 16:C:66:SER:HA     | 25:L:49:TYR:CE1   | 2.47                     | 0.50              |
| 17:D:10:A:OP2      | 24:K:131:THR:HG21 | 2.12                     | 0.50              |
| 17:D:36:C:C4       | 17:D:37:U:C5      | 3.00                     | 0.50              |
| 17:D:280:C:H1'     | 35:V:40:ARG:HH22  | 1.75                     | 0.50              |
| 17:D:339:C:C2      | 17:D:340:U:C5     | 2.99                     | 0.50              |
| 17:D:1439:G:P      | 18:E:33:LYS:NZ    | 2.82                     | 0.50              |
| 24:K:62:LYS:HA     | 24:K:62:LYS:HE3   | 1.93                     | 0.50              |
| 29:P:37:ARG:HB3    | 29:P:75:ASP:HB2   | 1.93                     | 0.50              |
| 32:S:87:ALA:HA     | 32:S:90:ARG:HG2   | 1.94                     | 0.50              |
| 37:X:71:ARG:HD2    | 37:X:72:GLU:N     | 2.26                     | 0.50              |
| 37:X:92:ARG:HD2    | 40:a:888:C:OP1    | 2.12                     | 0.50              |
| 40:a:234:U:C2      | 40:a:235:U:C6     | 3.00                     | 0.50              |
| 40:a:1945:G:C4     | 40:a:1946:U:C5    | 3.00                     | 0.50              |
| 40:a:1996:C:H5''   | 49:j:128:ARG:NH1  | 2.25                     | 0.50              |
| 40:a:2063:C:C2     | 40:a:2064:C:C6    | 3.00                     | 0.50              |
| 40:a:2065:C:H2'    | 40:a:2066:C:H6    | 1.77                     | 0.50              |
| 40:a:2179:C:C2     | 40:a:2180:U:C5    | 3.00                     | 0.50              |
| 46:g:47:LYS:NZ     | 53:n:115:ARG:HA   | 2.27                     | 0.50              |
| 50:k:34:LEU:CB     | 50:k:51:GLU:OE2   | 2.60                     | 0.50              |
| 55:p:137:ASP:OD2   | 55:p:140:VAL:HG23 | 2.12                     | 0.50              |
| 58:s:13:ARG:HH22   | 58:s:49:ASP:C     | 2.19                     | 0.50              |
| 61:v:50:ARG:CA     | 61:v:53:MET:SD    | 3.00                     | 0.50              |
| 62:w:58:ASP:CG     | 62:w:80:PHE:CZ    | 2.89                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1:36:LEU:HD23   | 2:1:48:LYS:HB2    | 1.93                     | 0.50              |
| 3:2:14:PRO:HA     | 3:2:32:LEU:HD13   | 1.94                     | 0.50              |
| 5:4:2:PHE:HB2     | 5:4:61:LEU:HG     | 1.94                     | 0.50              |
| 8:7:24:U:H2'      | 8:7:24:U:O2       | 2.12                     | 0.50              |
| 11:AA:93:SER:HA   | 11:AA:128:PRO:HA  | 1.92                     | 0.50              |
| 12:AB:19:GLU:HG2  | 12:AB:23:ARG:CZ   | 2.42                     | 0.50              |
| 14:AE:430:HIS:HB3 | 14:AE:925:GLU:HG3 | 1.93                     | 0.50              |
| 16:C:25:ASP:O     | 16:C:29:LEU:HD13  | 2.11                     | 0.50              |
| 17:D:136:C:C2     | 17:D:137:U:C6     | 3.00                     | 0.50              |
| 17:D:1071:C:H2'   | 17:D:1072:G:C8    | 2.47                     | 0.50              |
| 17:D:1492:A:O2'   | 17:D:1493:A:H5''  | 2.11                     | 0.50              |
| 20:G:38:VAL:HG22  | 21:H:75:VAL:HG21  | 1.92                     | 0.50              |
| 20:G:114:LEU:HD13 | 20:G:144:LEU:HB3  | 1.94                     | 0.50              |
| 24:K:113:ALA:CA   | 24:K:116:GLU:OE1  | 2.60                     | 0.50              |
| 25:L:66:ALA:HB1   | 25:L:67:PRO:HD2   | 1.94                     | 0.50              |
| 34:U:73:ALA:HA    | 34:U:76:LYS:CE    | 2.41                     | 0.50              |
| 40:a:16:C:O4'     | 48:i:15:MET:HE3   | 2.12                     | 0.50              |
| 40:a:594:U:H2'    | 40:a:595:C:C6     | 2.47                     | 0.50              |
| 40:a:2063:C:C4    | 40:a:2064:C:C5    | 3.00                     | 0.50              |
| 55:p:24:ILE:HG22  | 55:p:35:ARG:O     | 2.11                     | 0.50              |
| 6:5:9:DG:H5''     | 11:AA:473:ARG:HB3 | 0.54                     | 0.50              |
| 9:9:67:THR:N      | 9:9:68:PRO:CD     | 2.75                     | 0.50              |
| 9:9:87:GLU:OE2    | 9:9:95:LEU:HB2    | 2.12                     | 0.50              |
| 14:AE:425:ARG:NH1 | 14:AE:458:ASN:O   | 2.45                     | 0.50              |
| 14:AE:749:LYS:HD3 | 14:AE:753:SER:HB2 | 1.94                     | 0.50              |
| 16:C:12:ARG:HG3   | 21:H:264:GLU:CB   | 2.41                     | 0.50              |
| 17:D:555:U:H2'    | 17:D:556:C:C6     | 2.46                     | 0.50              |
| 17:D:736:C:H2'    | 17:D:737:C:H6     | 1.77                     | 0.50              |
| 17:D:821:G:H2'    | 17:D:822:U:C6     | 2.47                     | 0.50              |
| 17:D:1017:U:O2'   | 17:D:1018:G:O4'   | 2.30                     | 0.50              |
| 20:G:109:GLN:O    | 20:G:113:ARG:NE   | 2.45                     | 0.50              |
| 21:H:303:LEU:O    | 21:H:303:LEU:CG   | 2.60                     | 0.50              |
| 22:I:82:GLU:O     | 22:I:86:LYS:CD    | 2.60                     | 0.50              |
| 25:L:9:MET:O      | 25:L:84:VAL:HA    | 2.12                     | 0.50              |
| 25:L:35:LYS:HG3   | 25:L:36:ILE:N     | 2.27                     | 0.50              |
| 26:M:74:GLU:OE1   | 26:M:75:VAL:O     | 2.30                     | 0.50              |
| 27:N:35:ALA:O     | 27:N:39:VAL:HG23  | 2.12                     | 0.50              |
| 33:T:33:THR:OG1   | 33:T:63:ARG:NH1   | 2.45                     | 0.50              |
| 40:a:4:U:C2       | 40:a:5:A:C8       | 3.00                     | 0.50              |
| 40:a:69:C:O2      | 40:a:73:A:O2'     | 2.26                     | 0.50              |
| 40:a:672:C:O2'    | 51:l:77:ILE:HD11  | 2.11                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:a:1205:A:C2     | 51:l:165:HIS:CE1   | 3.00                     | 0.50              |
| 40:a:1348:C:O2     | 40:a:1348:C:H2'    | 2.11                     | 0.50              |
| 40:a:2290:G:H2'    | 40:a:2291:U:C6     | 2.47                     | 0.50              |
| 40:a:2362:C:O5'    | 54:o:40:ARG:NH2    | 2.45                     | 0.50              |
| 40:a:2489:U:H2'    | 40:a:2490:G:O4'    | 2.12                     | 0.50              |
| 40:a:2547:A:H2'    | 40:a:2548:U:H6     | 1.77                     | 0.50              |
| 47:h:131:PRO:HD3   | 47:h:189:ARG:NH1   | 2.27                     | 0.50              |
| 50:k:7:GLU:CG      | 50:k:27:LYS:HZ3    | 2.25                     | 0.50              |
| 53:n:122:PHE:CE2   | 53:n:128:TYR:CD1   | 3.00                     | 0.50              |
| 55:p:26:ILE:HG22   | 55:p:75:MET:HE2    | 1.94                     | 0.50              |
| 6:5:10:DT:N1       | 11:AA:62:TYR:HE2   | 2.07                     | 0.49              |
| 11:AA:400:VAL:HG21 | 11:AA:452:ARG:HE   | 1.77                     | 0.49              |
| 11:AA:812:PHE:O    | 14:AE:504:GLN:NE2  | 2.40                     | 0.49              |
| 14:AE:59:ALA:HB3   | 14:AE:71:LEU:CD2   | 2.42                     | 0.49              |
| 16:C:13:PHE:CB     | 16:C:51:TYR:CD1    | 2.95                     | 0.49              |
| 17:D:404:G:O2'     | 17:D:498:A:N1      | 2.38                     | 0.49              |
| 17:D:626:G:O3'     | 34:U:51:ARG:NH1    | 2.45                     | 0.49              |
| 17:D:653:U:O4'     | 27:N:56:LYS:CE     | 2.60                     | 0.49              |
| 17:D:1227:A:H5'    | 37:X:110:LYS:HZ1   | 1.77                     | 0.49              |
| 20:G:110:SER:CA    | 20:G:113:ARG:HE    | 2.25                     | 0.49              |
| 33:T:33:THR:HG21   | 33:T:85:LEU:HD12   | 1.94                     | 0.49              |
| 40:a:44:A:H2'      | 40:a:45:G:O4'      | 2.12                     | 0.49              |
| 40:a:851:C:H2'     | 40:a:852:U:C6      | 2.46                     | 0.49              |
| 40:a:1801:A:OP1    | 47:h:146:MET:HE1   | 2.11                     | 0.49              |
| 40:a:2159:G:H2'    | 40:a:2160:C:C6     | 2.47                     | 0.49              |
| 41:b:51:VAL:N      | 41:b:62:LYS:HZ3    | 2.10                     | 0.49              |
| 46:g:36:VAL:HG21   | 46:g:41:HIS:ND1    | 2.27                     | 0.49              |
| 47:h:160:THR:O     | 47:h:195:VAL:HG12  | 2.12                     | 0.49              |
| 51:l:97:ASN:ND2    | 51:l:100:MET:HE2   | 2.27                     | 0.49              |
| 57:r:90:LEU:HD21   | 57:r:94:ILE:CD1    | 2.42                     | 0.49              |
| 58:s:55:ILE:CG1    | 58:s:123:LYS:HE2   | 2.42                     | 0.49              |
| 61:v:41:LEU:HD22   | 61:v:45:GLN:NE2    | 2.27                     | 0.49              |
| 62:w:73:ASN:C      | 62:w:73:ASN:HD22   | 2.17                     | 0.49              |
| 9:9:108:VAL:O      | 9:9:109:LYS:HB3    | 2.12                     | 0.49              |
| 10:A:56:C:H2'      | 10:A:57:A:H5''     | 1.94                     | 0.49              |
| 11:AA:232:ILE:HG12 | 11:AA:237:LEU:HG   | 1.93                     | 0.49              |
| 12:AB:9:CYS:N      | 12:AB:53:ASN:HB3   | 2.24                     | 0.49              |
| 12:AB:29:LEU:HB3   | 12:AB:56:PHE:HD2   | 1.77                     | 0.49              |
| 13:AD:100:LEU:HB2  | 13:AD:144:ILE:HG23 | 1.94                     | 0.49              |
| 14:AE:107:LEU:HD22 | 14:AE:299:LEU:HD21 | 1.94                     | 0.49              |
| 16:C:51:TYR:HD1    | 16:C:54:GLN:HE22   | 1.58                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:C:73:ARG:HH12   | 30:Q:113:VAL:HB    | 1.76                     | 0.49              |
| 17:D:35:G:H2'      | 17:D:36:C:C6       | 2.47                     | 0.49              |
| 17:D:311:C:O5'     | 17:D:311:C:H6      | 1.94                     | 0.49              |
| 21:H:304:VAL:HG11  | 21:H:346:LEU:HB2   | 1.93                     | 0.49              |
| 22:I:77:ILE:HA     | 22:I:84:VAL:HG13   | 1.94                     | 0.49              |
| 23:J:104:ARG:NE    | 23:J:104:ARG:HA    | 2.27                     | 0.49              |
| 23:J:170:TRP:CD2   | 23:J:186:PRO:HB3   | 2.47                     | 0.49              |
| 24:K:88:VAL:HG12   | 24:K:93:ARG:HA     | 1.93                     | 0.49              |
| 38:Y:77:VAL:HG13   | 38:Y:81:LYS:NZ     | 2.27                     | 0.49              |
| 40:a:57:C:H2'      | 40:a:58:G:O4'      | 2.12                     | 0.49              |
| 40:a:235:U:C2      | 40:a:236:C:C5      | 3.00                     | 0.49              |
| 40:a:1791:A:C2     | 40:a:1829:A:O4'    | 2.65                     | 0.49              |
| 40:a:2193:G:O2'    | 40:a:2194:U:OP1    | 2.28                     | 0.49              |
| 58:s:98:GLU:HB3    | 58:s:102:GLU:OE2   | 2.12                     | 0.49              |
| 61:v:70:ASP:C      | 61:v:92:TRP:CZ3    | 2.90                     | 0.49              |
| 64:y:25:THR:OG1    | 64:y:88:ARG:HB3    | 2.12                     | 0.49              |
| 9:9:3:LEU:CD1      | 9:9:4:ASN:N        | 2.63                     | 0.49              |
| 10:A:15:G:H2'      | 10:A:15:G:N3       | 2.27                     | 0.49              |
| 11:AA:1340:GLU:HB2 | 14:AE:19:ALA:HB3   | 1.94                     | 0.49              |
| 14:AE:412:LEU:HD22 | 14:AE:441:LEU:HD21 | 1.94                     | 0.49              |
| 10:B:15:G:H2'      | 10:B:15:G:N3       | 2.27                     | 0.49              |
| 17:D:373:A:C2      | 17:D:482:A:C6      | 3.00                     | 0.49              |
| 17:D:376:G:OP2     | 34:U:70:ARG:HD3    | 2.13                     | 0.49              |
| 17:D:925:G:C6      | 17:D:927:G:N7      | 2.80                     | 0.49              |
| 17:D:953:G:O6      | 37:X:103:LYS:CE    | 2.60                     | 0.49              |
| 20:G:111:ILE:HD13  | 20:G:148:LEU:HD13  | 1.95                     | 0.49              |
| 24:K:34:THR:HG22   | 24:K:52:LYS:HD3    | 1.95                     | 0.49              |
| 24:K:46:VAL:N      | 24:K:71:MET:HE2    | 2.27                     | 0.49              |
| 24:K:134:ILE:O     | 24:K:137:VAL:HG12  | 2.12                     | 0.49              |
| 28:O:52:LEU:O      | 28:O:55:VAL:O      | 2.31                     | 0.49              |
| 31:R:38:TYR:HE2    | 31:R:40:THR:CG2    | 2.25                     | 0.49              |
| 40:a:251:A:OP1     | 60:u:58:TYR:OH     | 2.23                     | 0.49              |
| 40:a:532:A:N7      | 40:a:2021:C:O2'    | 2.44                     | 0.49              |
| 40:a:636:G:N2      | 60:u:76:GLU:OE2    | 2.45                     | 0.49              |
| 40:a:1036:G:C6     | 40:a:1120:G:C5     | 3.00                     | 0.49              |
| 45:f:3:LYS:HE2     | 45:f:3:LYS:HA      | 1.95                     | 0.49              |
| 47:h:124:ILE:C     | 47:h:125:LYS:HD3   | 2.36                     | 0.49              |
| 59:t:114:LYS:O     | 59:t:118:LEU:HD23  | 2.11                     | 0.49              |
| 62:w:103:ARG:HA    | 62:w:110:MET:HE2   | 1.93                     | 0.49              |
| 2:1:71:VAL:O       | 2:1:71:VAL:HG23    | 2.13                     | 0.49              |
| 9:9:52:MET:CE      | 9:9:85:SER:HB2     | 2.42                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:A:47:U:O2'      | 10:A:50:U:P        | 2.70                     | 0.49              |
| 11:AA:529:ARG:HH11 | 11:AA:572:ILE:HG22 | 1.77                     | 0.49              |
| 12:AB:146:ILE:O    | 29:P:100:ILE:HG22  | 2.11                     | 0.49              |
| 10:B:32:C:H2'      | 10:B:33:U:H5'      | 1.94                     | 0.49              |
| 17:D:922:G:H2'     | 17:D:923:A:C8      | 2.47                     | 0.49              |
| 17:D:1218:C:H2'    | 17:D:1219:A:C8     | 2.48                     | 0.49              |
| 17:D:1227:A:H5'    | 37:X:110:LYS:NZ    | 2.28                     | 0.49              |
| 24:K:157:ARG:HH12  | 27:N:43:GLU:CD     | 2.20                     | 0.49              |
| 27:N:83:LEU:HD11   | 31:R:4:VAL:HB      | 1.95                     | 0.49              |
| 29:P:7:ARG:HD3     | 29:P:75:ASP:CG     | 2.36                     | 0.49              |
| 37:X:3:ARG:HH22    | 46:g:36:VAL:HG12   | 1.77                     | 0.49              |
| 40:a:132:G:H2'     | 40:a:133:U:C6      | 2.47                     | 0.49              |
| 40:a:537:G:P       | 58:s:2:LYS:CE      | 3.00                     | 0.49              |
| 40:a:1199:U:H2'    | 40:a:1200:C:H6     | 1.77                     | 0.49              |
| 40:a:1607:C:N4     | 40:a:1622:G:OP2    | 2.35                     | 0.49              |
| 40:a:2349:G:O6     | 40:a:2369:A:N6     | 2.46                     | 0.49              |
| 40:a:2849:U:OP2    | 64:y:93:ARG:CZ     | 2.60                     | 0.49              |
| 40:a:2884:U:H3     | 48:i:40:ARG:NH1    | 2.09                     | 0.49              |
| 48:i:40:ARG:NH1    | 48:i:41:HIS:CD2    | 2.80                     | 0.49              |
| 55:p:94:TYR:CE1    | 55:p:152:ARG:HD2   | 2.48                     | 0.49              |
| 59:t:7:MET:SD      | 59:t:18:ARG:NE     | 2.85                     | 0.49              |
| 63:x:90:VAL:HG22   | 63:x:115:LEU:HD11  | 1.94                     | 0.49              |
| 64:y:9:GLU:HG3     | 64:y:55:LEU:CB     | 2.42                     | 0.49              |
| 65:z:74:ILE:HG13   | 65:z:78:LYS:HE3    | 1.94                     | 0.49              |
| 11:AA:143:ARG:NH1  | 11:AA:507:GLY:O    | 2.32                     | 0.49              |
| 11:AA:786:GLY:N    | 11:AA:789:THR:OG1  | 2.41                     | 0.49              |
| 12:AB:123:PHE:CZ   | 29:P:81:GLU:C      | 2.90                     | 0.49              |
| 12:AB:155:LYS:HG3  | 12:AB:156:ASN:N    | 2.25                     | 0.49              |
| 14:AE:287:ALA:HB3  | 14:AE:292:VAL:HG22 | 1.94                     | 0.49              |
| 14:AE:417:ARG:NH1  | 15:AF:43:ASN:O     | 2.45                     | 0.49              |
| 17:D:61:G:N7       | 18:E:6:SER:OG      | 2.33                     | 0.49              |
| 17:D:657:U:C1'     | 33:T:28:GLN:HE22   | 2.23                     | 0.49              |
| 21:H:342:ILE:HG12  | 21:H:344:LEU:HD12  | 1.93                     | 0.49              |
| 40:a:840:C:C2      | 40:a:841:G:C8      | 3.01                     | 0.49              |
| 40:a:1454:C:H4'    | 62:w:63:ARG:NH1    | 2.27                     | 0.49              |
| 40:a:1790:C:H2'    | 40:a:1791:A:C8     | 2.48                     | 0.49              |
| 40:a:2040:G:OP1    | 58:s:106:LYS:NZ    | 2.38                     | 0.49              |
| 40:a:2809:A:H2'    | 40:a:2810:A:C8     | 2.48                     | 0.49              |
| 47:h:141:VAL:HG23  | 47:h:162:VAL:HG12  | 1.94                     | 0.49              |
| 51:l:195:GLN:HA    | 51:l:198:GLU:OE1   | 2.13                     | 0.49              |
| 65:z:51:ARG:N      | 65:z:51:ARG:HD2    | 2.28                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:2:10:VAL:HG12    | 3:2:11:LEU:HD12    | 1.93                     | 0.49              |
| 7:6:19:DC:H2'      | 7:6:20:DA:C8       | 2.48                     | 0.49              |
| 8:7:23:U:O2        | 8:7:23:U:H5''      | 2.12                     | 0.49              |
| 9:9:25:ALA:CB      | 9:9:99:PHE:HD2     | 2.26                     | 0.49              |
| 9:9:43:LYS:HA      | 9:9:46:ARG:NH1     | 2.27                     | 0.49              |
| 12:AB:143:LEU:HD22 | 12:AB:145:LEU:HG   | 1.94                     | 0.49              |
| 14:AE:209:ASN:HB3  | 14:AE:214:ARG:HH21 | 1.77                     | 0.49              |
| 26:M:111:ARG:NH2   | 26:M:126:ASP:OD2   | 2.43                     | 0.49              |
| 27:N:110:VAL:C     | 27:N:111:MET:SD    | 2.95                     | 0.49              |
| 35:V:17:MET:HG3    | 35:V:20:SER:HB2    | 1.95                     | 0.49              |
| 35:V:42:THR:HG22   | 35:V:44:LEU:HD12   | 1.95                     | 0.49              |
| 40:a:3:U:C2        | 40:a:4:U:C5        | 3.00                     | 0.49              |
| 40:a:265:A:N1      | 40:a:427:U:O2'     | 2.40                     | 0.49              |
| 40:a:272:A:N3      | 40:a:273:G:C8      | 2.80                     | 0.49              |
| 40:a:583:G:OP1     | 65:z:11:ARG:NH2    | 2.46                     | 0.49              |
| 40:a:1843:C:C2     | 40:a:1844:C:C5     | 3.00                     | 0.49              |
| 40:a:2014:A:H2'    | 40:a:2015:A:C8     | 2.47                     | 0.49              |
| 40:a:2684:U:C4     | 40:a:2685:G:N7     | 2.81                     | 0.49              |
| 40:a:2754:U:O3'    | 56:q:19:ARG:NH2    | 2.46                     | 0.49              |
| 42:c:6:GLN:CD      | 42:c:49:LEU:HD22   | 2.38                     | 0.49              |
| 51:l:5:LEU:HD23    | 51:l:122:GLU:HG3   | 1.95                     | 0.49              |
| 51:l:141:MET:O     | 51:l:142:ALA:HB3   | 2.13                     | 0.49              |
| 55:p:94:TYR:C      | 55:p:95:ARG:HD2    | 2.38                     | 0.49              |
| 56:q:10:LEU:HD23   | 56:q:33:HIS:CD2    | 2.47                     | 0.49              |
| 58:s:73:VAL:CG1    | 58:s:74:TYR:N      | 2.75                     | 0.49              |
| 59:t:88:ASN:OD1    | 59:t:89:ASN:N      | 2.46                     | 0.49              |
| 61:v:57:VAL:HG22   | 61:v:60:GLN:O      | 2.13                     | 0.49              |
| 2:1:23:LEU:HD21    | 2:1:35:ILE:HG22    | 1.95                     | 0.49              |
| 12:AB:129:ILE:O    | 12:AB:142:LEU:HB3  | 2.12                     | 0.49              |
| 17:D:377:G:OP1     | 34:U:5:ARG:CZ      | 2.60                     | 0.49              |
| 17:D:406:G:C5      | 17:D:495:A:C5      | 3.01                     | 0.49              |
| 17:D:537:G:OP1     | 31:R:110:ARG:NH2   | 2.38                     | 0.49              |
| 17:D:610:U:O2      | 17:D:610:U:H2'     | 2.12                     | 0.49              |
| 17:D:816:A:OP1     | 17:D:1526:G:O2'    | 2.27                     | 0.49              |
| 20:G:23:TRP:CZ3    | 20:G:25:PRO:HA     | 2.47                     | 0.49              |
| 26:M:109:ARG:O     | 26:M:119:ARG:NH2   | 2.46                     | 0.49              |
| 30:Q:98:ARG:HG2    | 30:Q:98:ARG:HH11   | 1.78                     | 0.49              |
| 35:V:62:ARG:HA     | 35:V:73:TRP:CZ3    | 2.47                     | 0.49              |
| 37:X:81:MET:HG2    | 40:a:888:C:C4      | 2.47                     | 0.49              |
| 38:Y:126:ARG:HH12  | 40:a:1082:U:C3'    | 2.26                     | 0.49              |
| 40:a:1199:U:H2'    | 40:a:1200:C:C6     | 2.47                     | 0.49              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 40:a:2313:C:H5'' | 53:n:88:LYS:HD2     | 1.95                     | 0.49              |
| 40:a:2392:A:C8   | 40:a:2429:G:C2      | 3.00                     | 0.49              |
| 40:a:2485:G:O3'  | 61:v:125:PRO:HB3    | 2.12                     | 0.49              |
| 40:a:2682:A:C5'  | 49:j:11:MET:HE1     | 2.42                     | 0.49              |
| 40:a:2740:A:H2'  | 40:a:2741:A:C8      | 2.48                     | 0.49              |
| 40:a:2902:C:N4   | 40:a:2903:U:O4      | 2.45                     | 0.49              |
| 47:h:52:ARG:HG3  | 47:h:53:HIS:ND1     | 2.27                     | 0.49              |
| 47:h:261:LYS:HA  | 47:h:264:ASP:OD2    | 2.12                     | 0.49              |
| 53:n:8:TYR:HA    | 53:n:12:VAL:HB      | 1.95                     | 0.49              |
| 58:s:54:ILE:O    | 58:s:123:LYS:HG2    | 2.12                     | 0.49              |
| 64:y:7:GLN:NE2   | 64:y:10:GLN:HE21    | 2.11                     | 0.49              |
| 65:z:79:PHE:CE1  | 65:z:110:VAL:HG22   | 2.48                     | 0.49              |
| 3:2:2:ILE:HG12   | 3:2:42:GLU:CD       | 2.37                     | 0.49              |
| 5:4:35:GLU:OE1   | 5:4:93:ARG:NH2      | 2.46                     | 0.49              |
| 8:7:3:G:H5''     | 17:D:1501:C:N4      | 2.27                     | 0.49              |
| 11:AA:9:LYS:HG2  | 11:AA:1171:ARG:HH12 | 1.77                     | 0.49              |
| 10:B:68:C:C3'    | 10:B:69:C:H5''      | 2.42                     | 0.49              |
| 17:D:652:U:C3'   | 27:N:56:LYS:HZ1     | 2.19                     | 0.49              |
| 17:D:718:A:C8    | 30:Q:118:HIS:HB3    | 2.48                     | 0.49              |
| 17:D:1215:G:C2   | 17:D:1216:A:C8      | 3.01                     | 0.49              |
| 19:F:63:GLU:O    | 19:F:67:ARG:HD2     | 2.12                     | 0.49              |
| 21:H:267:TRP:CE3 | 21:H:340:ARG:HG3    | 2.47                     | 0.49              |
| 23:J:113:GLU:O   | 23:J:117:LEU:HG     | 2.13                     | 0.49              |
| 24:K:13:GLU:C    | 24:K:14:LYS:HD2     | 2.37                     | 0.49              |
| 28:O:12:ARG:HD3  | 28:O:13:LYS:H       | 1.78                     | 0.49              |
| 29:P:64:GLN:OE1  | 29:P:65:TYR:O       | 2.31                     | 0.49              |
| 34:U:18:GLN:NE2  | 34:U:35:ARG:HE      | 2.10                     | 0.49              |
| 35:V:42:THR:HG22 | 35:V:44:LEU:HD11    | 1.95                     | 0.49              |
| 40:a:1142:A:C4   | 40:a:1144:A:N7      | 2.80                     | 0.49              |
| 40:a:1590:A:H2'  | 40:a:1591:A:C8      | 2.48                     | 0.49              |
| 40:a:1800:C:HO2' | 40:a:1818:U:H3      | 1.61                     | 0.49              |
| 40:a:1808:A:O2'  | 42:c:3:ARG:NH1      | 2.46                     | 0.49              |
| 40:a:1932:A:H2'  | 40:a:1933:G:O4'     | 2.13                     | 0.49              |
| 40:a:2093:G:N7   | 40:a:2225:A:H2'     | 2.28                     | 0.49              |
| 46:g:63:ARG:HG3  | 46:g:64:PHE:CD1     | 2.48                     | 0.49              |
| 58:s:123:LYS:CE  | 58:s:132:HIS:HD2    | 2.25                     | 0.49              |
| 58:s:125:TYR:HE2 | 58:s:130:HIS:HB2    | 1.78                     | 0.49              |
| 60:u:77:ILE:HD11 | 60:u:108:ALA:HB1    | 1.95                     | 0.49              |
| 61:v:29:GLY:HA3  | 61:v:104:GLU:HG3    | 1.94                     | 0.49              |
| 9:9:67:THR:O     | 9:9:72:LEU:HG       | 2.12                     | 0.49              |
| 10:A:21:A:H4'    | 10:A:21:A:OP1       | 2.13                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:AA:411:ARG:NH2  | 11:AA:427:ASP:OD2 | 2.44                     | 0.49              |
| 12:AB:50:LEU:HD21  | 14:AE:285:LEU:HB3 | 1.93                     | 0.49              |
| 14:AE:67:ASP:C     | 14:AE:69:GLU:N    | 2.71                     | 0.49              |
| 14:AE:814:CYS:SG   | 14:AE:815:GLY:N   | 2.85                     | 0.49              |
| 14:AE:1289:ASN:ND2 | 14:AE:1300:ALA:O  | 2.46                     | 0.49              |
| 10:B:72:A:H2'      | 10:B:73:A:H5''    | 1.95                     | 0.49              |
| 17:D:56:U:H2'      | 17:D:57:G:C8      | 2.48                     | 0.49              |
| 17:D:563:A:N1      | 17:D:884:U:O4     | 2.46                     | 0.49              |
| 17:D:674:G:P       | 25:L:86:ARG:HH22  | 2.35                     | 0.49              |
| 17:D:739:C:O2      | 33:T:42:HIS:HE1   | 1.94                     | 0.49              |
| 17:D:1080:A:OP1    | 24:K:50:TYR:OH    | 2.28                     | 0.49              |
| 21:H:112:ILE:HA    | 21:H:121:THR:O    | 2.12                     | 0.49              |
| 26:M:132:GLY:O     | 26:M:136:LYS:NZ   | 2.45                     | 0.49              |
| 30:Q:31:ILE:HD12   | 30:Q:46:THR:HG22  | 1.94                     | 0.49              |
| 33:T:64:ARG:CZ     | 33:T:64:ARG:CB    | 2.90                     | 0.49              |
| 38:Y:20:SER:CB     | 38:Y:21:PRO:HD3   | 2.43                     | 0.49              |
| 38:Y:21:PRO:CB     | 38:Y:22:PRO:HD3   | 2.41                     | 0.49              |
| 38:Y:86:LYS:HD3    | 38:Y:86:LYS:O     | 2.11                     | 0.49              |
| 40:a:1385:A:O2'    | 40:a:1396:U:O2    | 2.31                     | 0.49              |
| 40:a:1792:G:H5''   | 47:h:204:VAL:HG23 | 1.95                     | 0.49              |
| 40:a:2515:C:H2'    | 40:a:2516:A:H8    | 1.78                     | 0.49              |
| 46:g:47:LYS:HE2    | 53:n:115:ARG:HA   | 1.95                     | 0.49              |
| 53:n:70:ALA:O      | 53:n:81:GLN:OE1   | 2.31                     | 0.49              |
| 62:w:114:GLU:N     | 62:w:114:GLU:OE1  | 2.46                     | 0.49              |
| 1:O:73:LYS:HE2     | 1:O:73:LYS:HA     | 1.95                     | 0.49              |
| 2:1:35:ILE:O       | 2:1:39:THR:HG23   | 2.12                     | 0.49              |
| 14:AE:74:LYS:NZ    | 29:P:89:ARG:HA    | 2.27                     | 0.49              |
| 14:AE:520:ALA:HB3  | 14:AE:546:ALA:HB2 | 1.95                     | 0.49              |
| 14:AE:693:VAL:HG21 | 14:AE:743:MET:HE3 | 1.93                     | 0.49              |
| 17:D:71:A:N1       | 17:D:100:G:C8     | 2.81                     | 0.49              |
| 17:D:373:A:C2      | 17:D:374:A:C8     | 3.01                     | 0.49              |
| 17:D:429:U:N3      | 17:D:431:A:N6     | 2.61                     | 0.49              |
| 17:D:744:C:H2'     | 17:D:745:G:H8     | 1.77                     | 0.49              |
| 17:D:829:G:O3'     | 20:G:23:TRP:HZ2   | 1.95                     | 0.49              |
| 20:G:49:MET:CE     | 20:G:201:PRO:CD   | 2.87                     | 0.49              |
| 22:I:164:ARG:HD2   | 22:I:166:GLU:OE2  | 2.12                     | 0.49              |
| 24:K:157:ARG:CZ    | 27:N:43:GLU:HG3   | 2.43                     | 0.49              |
| 31:R:80:ILE:HG22   | 31:R:81:LEU:N     | 2.27                     | 0.49              |
| 33:T:35:GLN:HB3    | 33:T:59:MET:HE1   | 1.95                     | 0.49              |
| 33:T:71:LYS:HE2    | 33:T:78:TYR:CE2   | 2.48                     | 0.49              |
| 34:U:12:LYS:HD3    | 34:U:13:LYS:HG2   | 1.93                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:a:26:G:H2'      | 40:a:27:G:O4'     | 2.13                     | 0.49              |
| 40:a:145:C:H2'     | 40:a:146:A:H8     | 1.77                     | 0.49              |
| 40:a:2351:G:O6     | 54:o:39:LYS:HE3   | 2.13                     | 0.49              |
| 45:f:41:THR:CA     | 45:f:45:ARG:HH22  | 2.25                     | 0.49              |
| 49:j:55:LYS:NZ     | 49:j:59:ARG:HB3   | 2.23                     | 0.49              |
| 55:p:69:ARG:NH1    | 55:p:73:ASN:HD21  | 2.11                     | 0.49              |
| 58:s:131:ASN:OD1   | 58:s:131:ASN:O    | 2.30                     | 0.49              |
| 59:t:59:LYS:HZ3    | 59:t:92:GLU:CG    | 2.26                     | 0.49              |
| 61:v:58:LYS:O      | 61:v:59:ARG:HG3   | 2.13                     | 0.49              |
| 62:w:82:GLU:O      | 62:w:86:ARG:HG2   | 2.13                     | 0.49              |
| 64:y:9:GLU:HG3     | 64:y:55:LEU:HB2   | 1.95                     | 0.49              |
| 2:1:95:ARG:NH1     | 2:1:97:LEU:HG     | 2.28                     | 0.48              |
| 4:3:6:ARG:NH1      | 40:a:84:A:H2'     | 2.28                     | 0.48              |
| 5:4:1:MET:SD       | 5:4:3:THR:OG1     | 2.71                     | 0.48              |
| 9:9:77:VAL:CG1     | 9:9:82:ILE:HG21   | 2.41                     | 0.48              |
| 11:AA:18:ARG:HE    | 11:AA:620:ASN:HA  | 1.77                     | 0.48              |
| 11:AA:400:VAL:HG11 | 11:AA:452:ARG:HD2 | 1.94                     | 0.48              |
| 12:AB:117:ILE:HG23 | 12:AB:160:ARG:O   | 2.13                     | 0.48              |
| 10:B:47:U:O2'      | 10:B:50:U:P       | 2.71                     | 0.48              |
| 17:D:908:A:H2'     | 17:D:909:A:C8     | 2.48                     | 0.48              |
| 17:D:1324:A:H2'    | 17:D:1325:C:H6    | 1.78                     | 0.48              |
| 17:D:1439:G:OP1    | 18:E:33:LYS:CE    | 2.61                     | 0.48              |
| 18:E:54:MET:HE1    | 18:E:75:HIS:HE1   | 1.77                     | 0.48              |
| 22:I:142:MET:HG3   | 22:I:170:GLU:OE1  | 2.13                     | 0.48              |
| 22:I:188:GLU:OE1   | 22:I:188:GLU:N    | 2.45                     | 0.48              |
| 26:M:108:ALA:O     | 26:M:119:ARG:NH2  | 2.45                     | 0.48              |
| 33:T:64:ARG:HA     | 33:T:64:ARG:HH11  | 1.75                     | 0.48              |
| 40:a:624:C:O2'     | 40:a:657:U:OP1    | 2.29                     | 0.48              |
| 40:a:1021:A:H3'    | 40:a:1021:A:N3    | 2.27                     | 0.48              |
| 40:a:1571:A:H2'    | 40:a:1572:A:C8    | 2.47                     | 0.48              |
| 40:a:1664:A:C2'    | 40:a:1665:A:H5'   | 2.43                     | 0.48              |
| 40:a:2420:C:C5'    | 50:k:8:LYS:NZ     | 2.76                     | 0.48              |
| 40:a:2591:C:H2'    | 40:a:2592:G:H8    | 1.78                     | 0.48              |
| 40:a:2677:G:C6     | 40:a:2731:G:C6    | 3.01                     | 0.48              |
| 44:e:2:LYS:HZ1     | 44:e:49:ASP:C     | 2.21                     | 0.48              |
| 49:j:101:PHE:CZ    | 49:j:203:VAL:HG12 | 2.48                     | 0.48              |
| 50:k:21:TYR:CE2    | 50:k:38:LYS:CG    | 2.96                     | 0.48              |
| 58:s:1:MET:HE2     | 65:z:97:ASP:OD2   | 2.13                     | 0.48              |
| 62:w:60:VAL:HG22   | 62:w:63:ARG:HH12  | 1.78                     | 0.48              |
| 4:3:94:ARG:CB      | 4:3:103:ILE:HD12  | 2.43                     | 0.48              |
| 11:AA:380:ALA:HA   | 12:AB:65:HIS:ND1  | 2.28                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:AA:732:ILE:HD11 | 11:AA:769:PRO:HB3 | 1.95                     | 0.48              |
| 10:B:22:G:O2'      | 10:B:23:C:O5'     | 2.31                     | 0.48              |
| 16:C:60:LYS:NZ     | 17:D:734:G:C3'    | 2.76                     | 0.48              |
| 17:D:43:C:P        | 34:U:12:LYS:NZ    | 2.86                     | 0.48              |
| 17:D:123:U:H5''    | 17:D:311:C:O2'    | 2.13                     | 0.48              |
| 17:D:977:A:O2'     | 17:D:979:C:OP2    | 2.25                     | 0.48              |
| 17:D:1319:A:C8     | 17:D:1323:G:C6    | 3.01                     | 0.48              |
| 18:E:22:ALA:HA     | 18:E:25:ARG:HE    | 1.78                     | 0.48              |
| 20:G:126:PHE:C     | 20:G:127:ASP:O    | 2.55                     | 0.48              |
| 22:I:134:MET:HE2   | 22:I:168:TYR:CG   | 2.49                     | 0.48              |
| 25:L:38:ARG:HD2    | 25:L:40:GLU:OE2   | 2.13                     | 0.48              |
| 26:M:138:ARG:HG2   | 26:M:142:HIS:CE1  | 2.48                     | 0.48              |
| 28:O:86:ALA:HA     | 28:O:89:GLU:HG2   | 1.95                     | 0.48              |
| 31:R:74:LEU:HD11   | 31:R:80:ILE:CD1   | 2.43                     | 0.48              |
| 36:W:44:MET:SD     | 36:W:62:VAL:CG1   | 2.99                     | 0.48              |
| 38:Y:60:VAL:CG2    | 38:Y:66:PHE:HB3   | 2.29                     | 0.48              |
| 40:a:15:G:C2'      | 48:i:15:MET:HE1   | 2.42                     | 0.48              |
| 40:a:807:U:OP2     | 60:u:41:ARG:NH1   | 2.42                     | 0.48              |
| 40:a:2193:G:HO2'   | 40:a:2194:U:P     | 2.36                     | 0.48              |
| 45:f:41:THR:N      | 45:f:45:ARG:NH2   | 2.61                     | 0.48              |
| 53:n:16:LEU:HD12   | 53:n:28:VAL:CG2   | 2.43                     | 0.48              |
| 53:n:67:ILE:HD13   | 53:n:87:CYS:HB3   | 1.95                     | 0.48              |
| 53:n:134:GLU:CG    | 53:n:137:ILE:HG23 | 2.40                     | 0.48              |
| 62:w:33:ILE:HD11   | 62:w:112:TYR:CE1  | 2.48                     | 0.48              |
| 62:w:35:LYS:NZ     | 62:w:112:TYR:CE2  | 2.76                     | 0.48              |
| 64:y:40:LEU:HD12   | 64:y:40:LEU:N     | 2.28                     | 0.48              |
| 5:4:77:VAL:HG13    | 5:4:77:VAL:O      | 2.14                     | 0.48              |
| 8:7:15:U:C2        | 15:AF:83:VAL:CG1  | 2.89                     | 0.48              |
| 10:A:22:G:O2'      | 10:A:23:C:O5'     | 2.31                     | 0.48              |
| 10:B:23:C:H2'      | 10:B:24:U:H6      | 1.77                     | 0.48              |
| 16:C:45:THR:HA     | 21:H:340:ARG:HH21 | 1.77                     | 0.48              |
| 17:D:331:G:H2'     | 18:E:4:ILE:HD11   | 1.95                     | 0.48              |
| 19:F:4:ILE:CD1     | 19:F:19:PHE:HA    | 2.43                     | 0.48              |
| 24:K:112:ARG:C     | 24:K:116:GLU:OE1  | 2.56                     | 0.48              |
| 25:L:62:MET:HE3    | 25:L:62:MET:CA    | 2.43                     | 0.48              |
| 27:N:96:MET:HG2    | 27:N:96:MET:O     | 2.13                     | 0.48              |
| 37:X:16:VAL:HG23   | 37:X:17:ILE:N     | 2.29                     | 0.48              |
| 40:a:39:G:H1'      | 51:l:43:THR:HG21  | 1.96                     | 0.48              |
| 40:a:208:C:H2'     | 40:a:209:C:H6     | 1.78                     | 0.48              |
| 40:a:379:G:N1      | 40:a:396:G:C6     | 2.82                     | 0.48              |
| 40:a:2189:U:O2'    | 40:a:2190:G:O5'   | 2.31                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:a:2455:G:H2'   | 40:a:2456:C:C6    | 2.48                     | 0.48              |
| 40:a:2771:C:C2    | 40:a:2772:C:C5    | 3.01                     | 0.48              |
| 41:b:45:PHE:HD2   | 41:b:80:ILE:HD11  | 1.77                     | 0.48              |
| 51:l:147:LEU:HD11 | 51:l:170:ARG:CD   | 2.43                     | 0.48              |
| 56:q:2:LYS:CE     | 56:q:35:GLN:HE21  | 2.25                     | 0.48              |
| 58:s:88:THR:O     | 58:s:92:MET:HE2   | 2.13                     | 0.48              |
| 59:t:1:MET:HE3    | 59:t:32:TYR:HB3   | 1.94                     | 0.48              |
| 60:u:117:THR:HG23 | 60:u:118:THR:N    | 2.28                     | 0.48              |
| 4:3:84:GLY:HA3    | 4:3:95:PHE:CZ     | 2.49                     | 0.48              |
| 9:9:31:ARG:HH22   | 40:a:1106:G:N2    | 2.10                     | 0.48              |
| 10:A:70:G:C3'     | 10:A:71:C:H5''    | 2.43                     | 0.48              |
| 12:AB:32:MET:HE2  | 12:AB:32:MET:HA   | 1.95                     | 0.48              |
| 12:AB:92:VAL:HG13 | 12:AB:96:LEU:O    | 2.13                     | 0.48              |
| 14:AE:977:SER:OG  | 14:AE:980:THR:OG1 | 2.31                     | 0.48              |
| 10:B:21:A:H4'     | 10:B:21:A:OP1     | 2.13                     | 0.48              |
| 16:C:60:LYS:CD    | 17:D:734:G:O2'    | 2.62                     | 0.48              |
| 17:D:718:A:C5     | 30:Q:118:HIS:ND1  | 2.81                     | 0.48              |
| 17:D:877:G:H5''   | 27:N:80:ARG:HD2   | 1.94                     | 0.48              |
| 22:I:119:SER:O    | 22:I:123:GLN:HG2  | 2.13                     | 0.48              |
| 23:J:62:ARG:NE    | 23:J:72:PHE:CE2   | 2.81                     | 0.48              |
| 24:K:16:ILE:H     | 24:K:16:ILE:HD12  | 1.79                     | 0.48              |
| 26:M:129:GLU:O    | 26:M:130:ASN:HB2  | 2.13                     | 0.48              |
| 28:O:32:GLN:HG3   | 28:O:32:GLN:O     | 2.13                     | 0.48              |
| 29:P:26:VAL:HG12  | 29:P:30:LYS:HZ2   | 1.77                     | 0.48              |
| 29:P:63:ASP:OD1   | 29:P:65:TYR:CZ    | 2.66                     | 0.48              |
| 33:T:5:THR:O      | 33:T:8:THR:OG1    | 2.27                     | 0.48              |
| 37:X:86:TYR:HE2   | 37:X:90:ARG:NH2   | 2.11                     | 0.48              |
| 40:a:6:A:O3'      | 58:s:132:HIS:CE1  | 2.67                     | 0.48              |
| 40:a:2061:G:C2    | 40:a:2063:C:C5    | 3.01                     | 0.48              |
| 40:a:2259:U:C2    | 40:a:2260:C:C5    | 3.01                     | 0.48              |
| 51:l:149:ILE:CG2  | 51:l:175:ILE:HD11 | 2.43                     | 0.48              |
| 64:y:13:MET:HG3   | 64:y:77:HIS:CE1   | 2.49                     | 0.48              |
| 2:1:1:MET:CG      | 2:1:62:ASP:OD2    | 2.61                     | 0.48              |
| 2:1:17:VAL:HG12   | 2:1:76:VAL:HG21   | 1.94                     | 0.48              |
| 11:AA:562:GLU:OE1 | 11:AA:662:SER:OG  | 2.28                     | 0.48              |
| 12:AB:6:LEU:O     | 12:AB:7:LEU:HD23  | 2.13                     | 0.48              |
| 13:AD:182:ARG:O   | 13:AD:205:MET:HA  | 2.14                     | 0.48              |
| 17:D:1314:C:H2'   | 17:D:1315:U:H6    | 1.78                     | 0.48              |
| 23:J:61:VAL:HA    | 23:J:64:ILE:HD12  | 1.96                     | 0.48              |
| 23:J:62:ARG:CZ    | 23:J:69:GLU:HG2   | 2.44                     | 0.48              |
| 23:J:170:TRP:CZ3  | 23:J:190:ASP:HB3  | 2.48                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 24:K:157:ARG:NH2   | 27:N:43:GLU:OE2     | 2.46                     | 0.48              |
| 25:L:70:VAL:O      | 25:L:74:LEU:CD2     | 2.56                     | 0.48              |
| 28:O:52:LEU:HB3    | 28:O:58:VAL:HG12    | 1.94                     | 0.48              |
| 29:P:5:ARG:HG3     | 29:P:7:ARG:HH12     | 1.78                     | 0.48              |
| 31:R:7:LEU:HD23    | 35:V:34:TYR:OH      | 2.12                     | 0.48              |
| 40:a:1141:U:H4'    | 40:a:1142:A:O5'     | 2.13                     | 0.48              |
| 40:a:1921:G:C2'    | 40:a:1922:G:H5'     | 2.43                     | 0.48              |
| 40:a:2685:G:OP1    | 59:t:78:ARG:NH2     | 2.47                     | 0.48              |
| 41:b:47:ALA:HB2    | 41:b:59:LEU:HD11    | 1.94                     | 0.48              |
| 43:d:117:G:OP1     | 63:x:56:LYS:HD3     | 2.14                     | 0.48              |
| 48:i:28:LEU:O      | 48:i:37:LYS:NZ      | 2.46                     | 0.48              |
| 48:i:40:ARG:NH1    | 48:i:41:HIS:CG      | 2.81                     | 0.48              |
| 53:n:22:TYR:HE2    | 53:n:29:PRO:HD3     | 1.79                     | 0.48              |
| 65:z:72:ASN:ND2    | 65:z:106:PHE:CE2    | 2.81                     | 0.48              |
| 4:3:28:VAL:HG23    | 4:3:34:VAL:HG12     | 1.96                     | 0.48              |
| 5:4:89:ILE:CG2     | 5:4:91:PHE:CE1      | 2.95                     | 0.48              |
| 9:9:31:ARG:NE      | 9:9:31:ARG:HA       | 2.28                     | 0.48              |
| 9:9:103:ASN:HA     | 9:9:107:GLU:HG3     | 1.96                     | 0.48              |
| 11:AA:836:LEU:HD13 | 11:AA:1054:LEU:HD13 | 1.95                     | 0.48              |
| 12:AB:51:PHE:CZ    | 14:AE:288:PRO:HG3   | 2.47                     | 0.48              |
| 17:D:429:U:O2      | 17:D:430:A:C8       | 2.66                     | 0.48              |
| 17:D:500:G:H2'     | 17:D:501:C:H6       | 1.77                     | 0.48              |
| 24:K:157:ARG:NH1   | 27:N:43:GLU:HA      | 2.29                     | 0.48              |
| 38:Y:74:PRO:O      | 38:Y:78:LEU:HG      | 2.13                     | 0.48              |
| 39:Z:29:LYS:HG3    | 39:Z:30:PHE:CE2     | 2.49                     | 0.48              |
| 40:a:760:G:H2'     | 40:a:761:A:O4'      | 2.14                     | 0.48              |
| 40:a:1825:U:P      | 47:h:52:ARG:NH1     | 2.86                     | 0.48              |
| 40:a:2012:G:H8     | 40:a:2012:G:O5'     | 1.96                     | 0.48              |
| 40:a:2043:C:C2     | 40:a:2044:C:C5      | 3.02                     | 0.48              |
| 40:a:2884:U:N3     | 48:i:40:ARG:NH1     | 2.62                     | 0.48              |
| 44:e:14:LEU:HD13   | 44:e:57:LEU:HD22    | 1.95                     | 0.48              |
| 50:k:7:GLU:HG2     | 50:k:27:LYS:NZ      | 2.29                     | 0.48              |
| 61:v:95:LEU:HD23   | 61:v:95:LEU:H       | 1.78                     | 0.48              |
| 65:z:58:ARG:HA     | 65:z:61:TRP:CE3     | 2.48                     | 0.48              |
| 6:5:17:DC:C5       | 11:AA:542:ARG:HD3   | 2.48                     | 0.48              |
| 10:A:32:C:H2'      | 10:A:33:U:H5'       | 1.94                     | 0.48              |
| 16:C:21:ILE:HG13   | 16:C:54:GLN:NE2     | 2.29                     | 0.48              |
| 16:C:65:LEU:HD23   | 16:C:67:LEU:HD11    | 1.96                     | 0.48              |
| 17:D:562:U:O3'     | 31:R:14:ARG:NH1     | 2.46                     | 0.48              |
| 17:D:1307:U:H2'    | 17:D:1308:U:C6      | 2.49                     | 0.48              |
| 19:F:62:ARG:HD2    | 19:F:63:GLU:N       | 2.29                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:G:131:LYS:HE3  | 20:G:132:LYS:NZ   | 2.29                     | 0.48              |
| 22:I:156:ARG:HG2  | 22:I:193:TYR:HB2  | 1.95                     | 0.48              |
| 25:L:65:GLU:OE1   | 25:L:65:GLU:HA    | 2.12                     | 0.48              |
| 29:P:15:HIS:O     | 29:P:18:ILE:HG22  | 2.14                     | 0.48              |
| 35:V:31:HIS:HD2   | 35:V:34:TYR:H     | 1.62                     | 0.48              |
| 37:X:9:ILE:HG13   | 37:X:10:PRO:HD2   | 1.95                     | 0.48              |
| 38:Y:99:LYS:NZ    | 38:Y:138:VAL:O    | 2.44                     | 0.48              |
| 40:a:6:A:N3       | 58:s:135:GLN:NE2  | 2.58                     | 0.48              |
| 40:a:67:U:N3      | 40:a:74:A:N6      | 2.62                     | 0.48              |
| 40:a:576:U:H2'    | 40:a:577:G:C8     | 2.48                     | 0.48              |
| 40:a:920:A:C5     | 40:a:921:C:C5     | 3.01                     | 0.48              |
| 40:a:1858:A:N6    | 40:a:1884:G:H1'   | 2.29                     | 0.48              |
| 40:a:2193:G:O2'   | 40:a:2194:U:P     | 2.72                     | 0.48              |
| 40:a:2314:A:C1'   | 53:n:155:THR:HG21 | 2.42                     | 0.48              |
| 49:j:124:ARG:HA   | 49:j:165:MET:CE   | 2.44                     | 0.48              |
| 50:k:19:HIS:CD2   | 50:k:20:PHE:N     | 2.82                     | 0.48              |
| 57:r:137:GLU:CG   | 57:r:138:VAL:HG23 | 2.39                     | 0.48              |
| 65:z:78:LYS:CD    | 65:z:117:LEU:HD21 | 2.43                     | 0.48              |
| 3:2:11:LEU:HD11   | 3:2:46:ALA:HB3    | 1.95                     | 0.48              |
| 3:2:69:ARG:HG3    | 3:2:74:ILE:HD13   | 1.96                     | 0.48              |
| 5:4:69:GLU:H      | 5:4:69:GLU:CD     | 2.22                     | 0.48              |
| 7:6:10:DG:OP1     | 14:AE:311:ARG:NH2 | 2.47                     | 0.48              |
| 9:9:24:SER:O      | 9:9:116:GLU:HB2   | 2.14                     | 0.48              |
| 9:9:52:MET:HE2    | 9:9:85:SER:HB2    | 1.95                     | 0.48              |
| 11:AA:554:HIS:HD2 | 11:AA:558:VAL:HB  | 1.77                     | 0.48              |
| 12:AB:112:PRO:HA  | 12:AB:133:PRO:HG2 | 1.96                     | 0.48              |
| 10:B:12:G:C2'     | 10:B:13:C:OP1     | 2.61                     | 0.48              |
| 17:D:123:U:C2     | 17:D:124:C:C5     | 3.01                     | 0.48              |
| 17:D:893:C:C2     | 17:D:894:G:C8     | 3.01                     | 0.48              |
| 17:D:1127:G:C2    | 17:D:1128:C:C6    | 3.01                     | 0.48              |
| 17:D:1172:C:H2'   | 17:D:1173:U:C6    | 2.49                     | 0.48              |
| 17:D:1314:C:H2'   | 17:D:1315:U:C6    | 2.48                     | 0.48              |
| 17:D:1530:G:H2'   | 17:D:1531:A:C8    | 2.49                     | 0.48              |
| 23:J:195:ILE:HG13 | 23:J:195:ILE:O    | 2.14                     | 0.48              |
| 33:T:77:ARG:HH21  | 33:T:80:GLN:NE2   | 2.11                     | 0.48              |
| 40:a:1042:G:C4    | 40:a:1043:C:C6    | 3.01                     | 0.48              |
| 40:a:1321:A:C5    | 40:a:1322:A:C8    | 3.02                     | 0.48              |
| 40:a:2537:U:H2'   | 40:a:2538:C:H6    | 1.79                     | 0.48              |
| 44:e:10:SER:OG    | 44:e:13:GLU:HG2   | 2.13                     | 0.48              |
| 51:l:40:ARG:HD2   | 51:l:92:HIS:CE1   | 2.48                     | 0.48              |
| 55:p:94:TYR:HD1   | 55:p:107:LEU:HD23 | 1.79                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 61:v:41:LEU:HG    | 61:v:96:ILE:HG13   | 1.95                     | 0.48              |
| 1:0:68:ARG:NH2    | 1:0:90:ARG:HD3     | 2.29                     | 0.48              |
| 9:9:97:LYS:HZ1    | 9:9:130:PRO:HA     | 1.77                     | 0.48              |
| 9:9:99:PHE:O      | 9:9:103:ASN:OD1    | 2.32                     | 0.48              |
| 10:A:26:G:H1      | 10:A:44:A:N6       | 2.12                     | 0.48              |
| 10:A:72:A:H2'     | 10:A:73:A:H5''     | 1.95                     | 0.48              |
| 14:AE:77:ARG:HA   | 14:AE:77:ARG:CZ    | 2.44                     | 0.48              |
| 14:AE:291:ILE:O   | 14:AE:293:ARG:N    | 2.46                     | 0.48              |
| 14:AE:429:LEU:HB3 | 14:AE:925:GLU:HG2  | 1.95                     | 0.48              |
| 14:AE:678:ARG:NH1 | 14:AE:756:GLU:OE1  | 2.46                     | 0.48              |
| 17:D:106:C:N4     | 18:E:10:ARG:HH22   | 2.12                     | 0.48              |
| 17:D:330:C:O2     | 17:D:330:C:H2'     | 2.14                     | 0.48              |
| 18:E:19:LYS:CG    | 18:E:20:HIS:N      | 2.76                     | 0.48              |
| 20:G:110:SER:CA   | 20:G:113:ARG:HH21  | 2.27                     | 0.48              |
| 22:I:134:MET:HG3  | 22:I:151:VAL:CG2   | 2.44                     | 0.48              |
| 26:M:71:PRO:HG3   | 26:M:103:TRP:HH2   | 1.76                     | 0.48              |
| 28:O:49:ARG:C     | 28:O:53:GLU:OE1    | 2.57                     | 0.48              |
| 28:O:118:LEU:HD22 | 28:O:123:ARG:C     | 2.39                     | 0.48              |
| 35:V:11:ARG:HD2   | 35:V:56:GLY:C      | 2.39                     | 0.48              |
| 35:V:50:ASN:HB2   | 35:V:52:GLU:OE2    | 2.13                     | 0.48              |
| 38:Y:126:ARG:NH1  | 40:a:1082:U:O5'    | 2.46                     | 0.48              |
| 40:a:962:G:C5     | 40:a:963:U:C5      | 3.01                     | 0.48              |
| 40:a:2327:A:H2'   | 40:a:2328:A:C8     | 2.49                     | 0.48              |
| 42:c:67:VAL:HA    | 42:c:70:GLU:OE1    | 2.14                     | 0.48              |
| 58:s:98:GLU:OE1   | 58:s:124:VAL:HG13  | 2.13                     | 0.48              |
| 62:w:37:THR:HG21  | 62:w:40:LYS:HZ2    | 1.79                     | 0.48              |
| 1:0:61:ALA:HB1    | 1:0:96:VAL:CG2     | 2.43                     | 0.48              |
| 2:1:23:LEU:HD21   | 2:1:35:ILE:CG2     | 2.44                     | 0.48              |
| 10:A:65:C:C2'     | 10:A:66:C:H5'      | 2.44                     | 0.48              |
| 11:AA:618:GLN:HG3 | 14:AE:770:LEU:HD13 | 1.95                     | 0.48              |
| 12:AB:141:LEU:O   | 12:AB:151:LYS:N    | 2.46                     | 0.48              |
| 16:C:60:LYS:NZ    | 17:D:735:C:C4'     | 2.74                     | 0.48              |
| 17:D:72:A:C5      | 17:D:73:C:C5       | 3.02                     | 0.48              |
| 17:D:1397:C:OP1   | 17:D:1397:C:H2'    | 2.13                     | 0.48              |
| 20:G:112:LYS:HE2  | 20:G:112:LYS:HA    | 1.94                     | 0.48              |
| 23:J:138:SER:O    | 23:J:139:PRO:C     | 2.57                     | 0.48              |
| 25:L:9:MET:HE2    | 25:L:51:ILE:CD1    | 2.44                     | 0.48              |
| 27:N:40:LEU:O     | 27:N:44:GLY:N      | 2.47                     | 0.48              |
| 32:S:12:LYS:HD2   | 32:S:16:LEU:CD2    | 2.44                     | 0.48              |
| 40:a:272:A:C2     | 40:a:273:G:C5      | 3.02                     | 0.48              |
| 40:a:984:A:N3     | 40:a:984:A:H2'     | 2.29                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:a:1666:G:H1'   | 59:t:3:GLN:NE2     | 2.29                     | 0.48              |
| 49:j:91:THR:HB    | 49:j:94:GLN:CG     | 2.44                     | 0.48              |
| 52:m:25:LYS:HE2   | 52:m:28:ARG:HH21   | 1.78                     | 0.48              |
| 5:4:1:MET:O       | 5:4:1:MET:HE3      | 2.13                     | 0.47              |
| 9:9:95:LEU:HD12   | 9:9:99:PHE:CZ      | 2.49                     | 0.47              |
| 10:A:12:G:C2'     | 10:A:13:C:OP1      | 2.61                     | 0.47              |
| 12:AB:50:LEU:HD21 | 14:AE:285:LEU:CB   | 2.44                     | 0.47              |
| 14:AE:87:LYS:HZ3  | 29:P:89:ARG:CZ     | 2.27                     | 0.47              |
| 14:AE:290:ILE:O   | 14:AE:290:ILE:HG12 | 2.14                     | 0.47              |
| 10:B:70:G:C3'     | 10:B:71:C:H5''     | 2.44                     | 0.47              |
| 17:D:109:A:C6     | 17:D:326:G:C6      | 3.02                     | 0.47              |
| 17:D:1428:A:H2'   | 17:D:1429:A:O4'    | 2.13                     | 0.47              |
| 19:F:33:ARG:O     | 19:F:36:GLU:HG2    | 2.14                     | 0.47              |
| 25:L:36:ILE:HD12  | 25:L:63:ASN:O      | 2.14                     | 0.47              |
| 30:Q:94:GLU:O     | 30:Q:97:ILE:HG22   | 2.13                     | 0.47              |
| 32:S:57:PRO:HA    | 32:S:60:GLN:OE1    | 2.13                     | 0.47              |
| 33:T:29:VAL:HG22  | 33:T:66:LEU:HD23   | 1.96                     | 0.47              |
| 37:X:86:TYR:CE2   | 37:X:90:ARG:NE     | 2.82                     | 0.47              |
| 37:X:94:GLY:C     | 37:X:95:LEU:HD22   | 2.38                     | 0.47              |
| 38:Y:19:PRO:HG2   | 38:Y:24:GLY:H      | 1.79                     | 0.47              |
| 40:a:654:A:N6     | 54:o:19:LYS:HD2    | 2.29                     | 0.47              |
| 40:a:783:A:N3     | 40:a:783:A:H2'     | 2.29                     | 0.47              |
| 40:a:2298:A:C4    | 40:a:2321:U:H5     | 2.31                     | 0.47              |
| 40:a:2298:A:H5''  | 53:n:72:LYS:CE     | 2.44                     | 0.47              |
| 40:a:2299:U:P     | 53:n:72:LYS:HE2    | 2.54                     | 0.47              |
| 40:a:2419:U:O2'   | 40:a:2420:C:H5'    | 2.14                     | 0.47              |
| 46:g:5:ILE:CD1    | 53:n:64:LYS:CE     | 2.92                     | 0.47              |
| 47:h:130:LEU:HG   | 47:h:135:ILE:HG13  | 1.96                     | 0.47              |
| 51:l:119:ILE:O    | 51:l:188:MET:N     | 2.35                     | 0.47              |
| 53:n:38:MET:HE3   | 53:n:57:LEU:HG     | 1.96                     | 0.47              |
| 61:v:29:GLY:H     | 61:v:104:GLU:HG2   | 1.79                     | 0.47              |
| 61:v:41:LEU:HD22  | 61:v:45:GLN:HE22   | 1.78                     | 0.47              |
| 61:v:42:THR:HA    | 61:v:93:VAL:HG12   | 1.95                     | 0.47              |
| 61:v:53:MET:HB2   | 61:v:116:ALA:HB1   | 1.96                     | 0.47              |
| 2:1:20:VAL:O      | 2:1:23:LEU:HB3     | 2.13                     | 0.47              |
| 2:1:25:ARG:HH12   | 40:a:520:G:P       | 2.37                     | 0.47              |
| 2:1:95:ARG:NH1    | 2:1:97:LEU:CD2     | 2.77                     | 0.47              |
| 10:A:35:A:H2'     | 10:A:36:U:C6       | 2.49                     | 0.47              |
| 10:A:75:C:O2'     | 10:A:76:A:N7       | 2.48                     | 0.47              |
| 11:AA:560:PRO:O   | 14:AE:780:ARG:NH2  | 2.47                     | 0.47              |
| 12:AB:2:GLN:HB2   | 12:AB:60:ASP:HB2   | 1.95                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AB:7:LEU:HD22   | 12:AB:78:PHE:HA    | 1.96                     | 0.47              |
| 14:AE:437:PHE:HZ   | 14:AE:453:VAL:HG11 | 1.79                     | 0.47              |
| 10:B:35:A:H2'      | 10:B:36:U:C6       | 2.49                     | 0.47              |
| 17:D:636:U:H5'     | 35:V:6:ARG:NE      | 2.29                     | 0.47              |
| 17:D:1149:C:H2'    | 17:D:1150:A:H8     | 1.79                     | 0.47              |
| 17:D:1308:U:H3'    | 37:X:98:ARG:NH2    | 2.29                     | 0.47              |
| 19:F:25:LYS:NZ     | 21:H:336:ASP:CG    | 2.68                     | 0.47              |
| 20:G:26:LYS:O      | 20:G:26:LYS:HD3    | 2.14                     | 0.47              |
| 23:J:76:TYR:CE2    | 23:J:204:TYR:CB    | 2.95                     | 0.47              |
| 23:J:124:MET:HE2   | 23:J:128:ARG:CA    | 2.43                     | 0.47              |
| 23:J:139:PRO:N     | 23:J:182:PHE:HE2   | 2.12                     | 0.47              |
| 24:K:57:PRO:HA     | 24:K:60:ILE:HG12   | 1.96                     | 0.47              |
| 26:M:135:VAL:HG23  | 26:M:136:LYS:HD2   | 1.96                     | 0.47              |
| 32:S:74:LEU:HD23   | 32:S:77:PHE:CD2    | 2.49                     | 0.47              |
| 36:W:33:THR:HG21   | 36:W:49:ILE:HD11   | 1.94                     | 0.47              |
| 38:Y:99:LYS:CD     | 38:Y:138:VAL:O     | 2.61                     | 0.47              |
| 40:a:208:C:C2      | 40:a:209:C:C5      | 3.01                     | 0.47              |
| 40:a:1048:A:C4     | 40:a:1049:C:C5     | 3.02                     | 0.47              |
| 40:a:1333:G:C2     | 40:a:1334:G:C8     | 3.03                     | 0.47              |
| 40:a:1349:C:N3     | 40:a:1350:C:C5     | 2.83                     | 0.47              |
| 40:a:1830:C:N3     | 40:a:1831:G:N7     | 2.61                     | 0.47              |
| 40:a:2373:G:H2'    | 40:a:2374:C:C6     | 2.49                     | 0.47              |
| 46:g:47:LYS:HE2    | 53:n:115:ARG:CZ    | 2.44                     | 0.47              |
| 50:k:25:LYS:HD3    | 50:k:51:GLU:OE2    | 2.14                     | 0.47              |
| 51:l:42:GLY:HA3    | 51:l:92:HIS:CE1    | 2.49                     | 0.47              |
| 53:n:93:GLY:C      | 53:n:97:TRP:CZ3    | 2.92                     | 0.47              |
| 55:p:9:VAL:HG23    | 55:p:69:ARG:HD2    | 1.95                     | 0.47              |
| 58:s:123:LYS:HD2   | 58:s:132:HIS:HD2   | 1.78                     | 0.47              |
| 59:t:20:MET:HB3    | 59:t:44:LYS:HE2    | 1.95                     | 0.47              |
| 59:t:20:MET:H      | 59:t:44:LYS:HZ3    | 1.62                     | 0.47              |
| 60:u:59:ARG:HH11   | 60:u:59:ARG:HG3    | 1.78                     | 0.47              |
| 63:x:41:ALA:HB2    | 63:x:48:LEU:HD11   | 1.95                     | 0.47              |
| 2:1:28:LYS:HB2     | 2:1:31:GLN:OE1     | 2.14                     | 0.47              |
| 5:4:59:GLU:OE1     | 5:4:59:GLU:N       | 2.47                     | 0.47              |
| 11:AA:1280:ALA:HB1 | 14:AE:918:ILE:HG22 | 1.95                     | 0.47              |
| 17:D:110:C:H2'     | 17:D:111:G:O4'     | 2.14                     | 0.47              |
| 17:D:808:C:OP1     | 33:T:48:LYS:HE3    | 2.14                     | 0.47              |
| 17:D:1227:A:C2     | 17:D:1228:C:C6     | 3.02                     | 0.47              |
| 17:D:1412:C:H2'    | 17:D:1413:A:C8     | 2.49                     | 0.47              |
| 24:K:157:ARG:NH1   | 27:N:43:GLU:CD     | 2.72                     | 0.47              |
| 26:M:109:ARG:C     | 26:M:119:ARG:HH21  | 2.23                     | 0.47              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 26:M:142:HIS:O   | 26:M:146:GLU:HG2   | 2.13                     | 0.47              |
| 27:N:34:VAL:HG22 | 27:N:59:LEU:HD21   | 1.96                     | 0.47              |
| 28:O:21:ILE:HD12 | 28:O:86:ALA:HB1    | 1.96                     | 0.47              |
| 31:R:2:ALA:N     | 31:R:7:LEU:HD11    | 2.29                     | 0.47              |
| 34:U:26:ASN:ND2  | 34:U:31:ARG:HE     | 2.11                     | 0.47              |
| 37:X:5:ALA:HB3   | 37:X:66:GLU:OE2    | 2.14                     | 0.47              |
| 40:a:1083:U:O2'  | 40:a:1085:A:OP2    | 2.32                     | 0.47              |
| 40:a:2246:G:H2'  | 40:a:2247:A:C8     | 2.49                     | 0.47              |
| 40:a:2296:U:H4'  | 40:a:2297:A:OP1    | 2.14                     | 0.47              |
| 40:a:2788:C:H2'  | 40:a:2789:C:C6     | 2.50                     | 0.47              |
| 40:a:2814:A:C4   | 40:a:2815:C:C5     | 3.03                     | 0.47              |
| 41:b:26:PHE:H    | 41:b:29:GLU:HG3    | 1.79                     | 0.47              |
| 46:g:45:THR:O    | 46:g:49:ARG:CZ     | 2.62                     | 0.47              |
| 58:s:15:TRP:HD1  | 58:s:53:TYR:HB2    | 1.78                     | 0.47              |
| 62:w:38:LEU:N    | 62:w:39:PRO:CD     | 2.76                     | 0.47              |
| 8:7:26:A:H3'     | 14:AE:395:LYS:NZ   | 2.29                     | 0.47              |
| 9:9:16:SER:HB2   | 9:9:20:LYS:NZ      | 2.29                     | 0.47              |
| 9:9:51:TYR:CD2   | 9:9:88:HIS:HB2     | 2.49                     | 0.47              |
| 10:A:33:U:H4'    | 26:M:84:THR:HB     | 1.96                     | 0.47              |
| 11:AA:565:GLU:HA | 11:AA:569:ILE:HG12 | 1.95                     | 0.47              |
| 12:AB:155:LYS:CG | 12:AB:156:ASN:H    | 2.26                     | 0.47              |
| 14:AE:74:LYS:HZ3 | 29:P:89:ARG:CG     | 2.27                     | 0.47              |
| 14:AE:79:LYS:CB  | 14:AE:81:ARG:HH12  | 2.28                     | 0.47              |
| 17:D:378:G:H2'   | 17:D:379:C:C6      | 2.49                     | 0.47              |
| 17:D:687:A:C2    | 17:D:704:A:C4      | 3.02                     | 0.47              |
| 17:D:1176:A:H2'  | 17:D:1177:G:O4'    | 2.14                     | 0.47              |
| 17:D:1325:C:C2   | 17:D:1326:U:C5     | 3.02                     | 0.47              |
| 28:O:49:ARG:O    | 28:O:53:GLU:OE1    | 2.32                     | 0.47              |
| 30:Q:85:MET:HB3  | 30:Q:113:VAL:HG11  | 1.95                     | 0.47              |
| 31:R:99:ARG:NE   | 31:R:104:CYS:SG    | 2.87                     | 0.47              |
| 36:W:9:PRO:HD3   | 46:g:64:PHE:CD2    | 2.49                     | 0.47              |
| 38:Y:52:LEU:O    | 38:Y:54:ILE:HG12   | 2.14                     | 0.47              |
| 39:Z:26:MET:O    | 39:Z:30:PHE:HB2    | 2.14                     | 0.47              |
| 40:a:581:C:C2    | 40:a:582:A:C8      | 3.02                     | 0.47              |
| 40:a:689:A:H2'   | 40:a:690:G:C8      | 2.49                     | 0.47              |
| 40:a:1794:A:H2'  | 40:a:1795:C:H6     | 1.80                     | 0.47              |
| 40:a:1841:U:C2   | 40:a:1842:G:C8     | 3.02                     | 0.47              |
| 40:a:2297:A:N1   | 40:a:2321:U:O4     | 2.47                     | 0.47              |
| 51:l:23:PHE:CE2  | 51:l:25:GLU:HA     | 2.50                     | 0.47              |
| 55:p:18:LYS:HE2  | 55:p:18:LYS:HA     | 1.96                     | 0.47              |
| 56:q:1:MET:CA    | 56:q:1:MET:HE3     | 2.43                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:v:53:MET:SD     | 61:v:53:MET:N      | 2.86                     | 0.47              |
| 61:v:59:ARG:CZ     | 61:v:59:ARG:O      | 2.63                     | 0.47              |
| 61:v:97:GLN:H      | 61:v:100:LYS:NZ    | 2.13                     | 0.47              |
| 63:x:115:LEU:HD23  | 63:x:117:PHE:HE1   | 1.79                     | 0.47              |
| 1:0:6:GLN:OE1      | 1:0:11:GLN:HG2     | 2.14                     | 0.47              |
| 4:3:40:ASN:OD1     | 4:3:65:ILE:HB      | 2.14                     | 0.47              |
| 5:4:11:GLU:OE2     | 5:4:19:ARG:NH2     | 2.47                     | 0.47              |
| 8:7:21:U:C3'       | 8:7:21:U:C6        | 2.97                     | 0.47              |
| 8:7:27:U:H3'       | 8:7:27:U:O2        | 2.15                     | 0.47              |
| 9:9:38:MET:SD      | 38:Y:117:THR:CG2   | 3.02                     | 0.47              |
| 10:A:19:G:C6       | 40:a:2112:G:O5'    | 2.67                     | 0.47              |
| 11:AA:363:LEU:HB3  | 11:AA:381:ALA:HB1  | 1.96                     | 0.47              |
| 11:AA:1286:THR:O   | 11:AA:1290:MET:HB2 | 2.14                     | 0.47              |
| 12:AB:131:THR:HG23 | 12:AB:142:LEU:HD22 | 1.97                     | 0.47              |
| 14:AE:804:ALA:O    | 14:AE:806:ASP:N    | 2.47                     | 0.47              |
| 10:B:30:G:O2'      | 10:B:31:G:H5'      | 2.15                     | 0.47              |
| 17:D:61:G:O6       | 18:E:10:ARG:NH2    | 2.47                     | 0.47              |
| 17:D:520:A:O2'     | 31:R:70:GLU:CD     | 2.58                     | 0.47              |
| 17:D:977:A:H1'     | 17:D:982:U:O4      | 2.15                     | 0.47              |
| 21:H:5:PHE:CE1     | 21:H:9:PHE:HE1     | 2.31                     | 0.47              |
| 22:I:25:ASN:O      | 22:I:27:LYS:N      | 2.47                     | 0.47              |
| 24:K:148:ASN:ND2   | 24:K:153:VAL:CG1   | 2.77                     | 0.47              |
| 26:M:71:PRO:O      | 26:M:96:ARG:NH1    | 2.47                     | 0.47              |
| 32:S:63:ARG:HD3    | 32:S:68:GLY:O      | 2.15                     | 0.47              |
| 35:V:30:LYS:HD3    | 35:V:35:GLY:HA2    | 1.97                     | 0.47              |
| 40:a:247:G:H4'     | 40:a:386:G:C5      | 2.49                     | 0.47              |
| 40:a:600:G:H2'     | 40:a:601:C:C6      | 2.49                     | 0.47              |
| 40:a:1197:G:C4     | 40:a:1198:U:C5     | 3.02                     | 0.47              |
| 40:a:1770:G:C6     | 40:a:1983:G:C5     | 3.03                     | 0.47              |
| 40:a:2070:A:H2'    | 40:a:2071:A:O4'    | 2.14                     | 0.47              |
| 51:l:112:LEU:CD1   | 51:l:117:ARG:HB2   | 2.39                     | 0.47              |
| 56:q:14:CYS:SG     | 56:q:33:HIS:HB3    | 2.53                     | 0.47              |
| 58:s:13:ARG:NH2    | 58:s:50:THR:HA     | 2.27                     | 0.47              |
| 58:s:39:LYS:HA     | 58:s:44:TYR:HD1    | 1.78                     | 0.47              |
| 63:x:115:LEU:HD23  | 63:x:117:PHE:CE1   | 2.49                     | 0.47              |
| 65:z:53:ARG:HG2    | 65:z:57:PHE:CE2    | 2.49                     | 0.47              |
| 5:4:2:PHE:CE1      | 5:4:56:PHE:CZ      | 3.03                     | 0.47              |
| 13:AC:64:VAL:HG11  | 13:AC:78:ILE:HG21  | 1.97                     | 0.47              |
| 13:AC:102:LEU:HD12 | 13:AC:115:ILE:HG12 | 1.96                     | 0.47              |
| 14:AE:87:LYS:NZ    | 29:P:89:ARG:CZ     | 2.78                     | 0.47              |
| 10:B:26:G:H1       | 10:B:44:A:N6       | 2.12                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 16:C:38:LYS:HA      | 16:C:38:LYS:CE      | 2.37                     | 0.47              |
| 17:D:311:C:P        | 34:U:31:ARG:NH2     | 2.86                     | 0.47              |
| 17:D:1149:C:C2      | 17:D:1150:A:C8      | 3.03                     | 0.47              |
| 17:D:1225:A:H2'     | 17:D:1226:C:C5      | 2.49                     | 0.47              |
| 17:D:1308:U:P       | 37:X:98:ARG:CG      | 3.03                     | 0.47              |
| 20:G:110:SER:HA     | 20:G:113:ARG:NE     | 2.29                     | 0.47              |
| 20:G:117:LEU:HD21   | 20:G:141:LEU:HB2    | 1.96                     | 0.47              |
| 33:T:77:ARG:NH2     | 33:T:80:GLN:NE2     | 2.62                     | 0.47              |
| 38:Y:126:ARG:NH1    | 40:a:1083:U:OP2     | 2.47                     | 0.47              |
| 40:a:591:U:C2       | 40:a:592:A:C8       | 3.03                     | 0.47              |
| 40:a:963:U:H2'      | 40:a:964:C:H6       | 1.79                     | 0.47              |
| 40:a:1385:A:C4      | 40:a:1386:C:C5      | 3.02                     | 0.47              |
| 40:a:1708:C:H2'     | 40:a:1709:U:H6      | 1.79                     | 0.47              |
| 40:a:1818:U:H6      | 47:h:156:ARG:NH2    | 2.13                     | 0.47              |
| 40:a:2091:C:O2      | 42:c:34:HIS:CE1     | 2.67                     | 0.47              |
| 40:a:2243:U:H2'     | 40:a:2244:U:H6      | 1.80                     | 0.47              |
| 45:f:41:THR:O       | 45:f:42:PRO:C       | 2.58                     | 0.47              |
| 47:h:205:LEU:HD12   | 47:h:210:ALA:CB     | 2.44                     | 0.47              |
| 48:i:4:GLN:OE1      | 48:i:8:PRO:CD       | 2.63                     | 0.47              |
| 51:l:168:ASP:HB3    | 51:l:183:PHE:CE2    | 2.49                     | 0.47              |
| 57:r:18:GLN:HE22    | 57:r:39:ALA:HB2     | 1.78                     | 0.47              |
| 59:t:42:THR:CG2     | 59:t:44:LYS:HZ1     | 2.27                     | 0.47              |
| 1:0:82:HIS:CD2      | 60:u:23:ILE:HG12    | 2.50                     | 0.47              |
| 2:1:11:ARG:CZ       | 2:1:11:ARG:HB3      | 2.45                     | 0.47              |
| 3:2:1:MET:HE1       | 40:a:139:U:C4       | 2.50                     | 0.47              |
| 5:4:48:MET:HE3      | 5:4:85:LYS:HA       | 1.97                     | 0.47              |
| 8:7:8:U:OP2         | 17:D:1397:C:O2      | 2.33                     | 0.47              |
| 10:A:30:G:O2'       | 10:A:31:G:H5'       | 2.15                     | 0.47              |
| 11:AA:848:GLU:HG2   | 11:AA:888:THR:HG22  | 1.96                     | 0.47              |
| 11:AA:1314:GLN:HB2  | 15:AF:28:ARG:HH12   | 1.79                     | 0.47              |
| 12:AB:111:TYR:HB3   | 12:AB:112:PRO:HD2   | 1.96                     | 0.47              |
| 12:AB:145:LEU:CD2   | 29:P:88:MET:SD      | 3.00                     | 0.47              |
| 14:AE:616:PRO:HA    | 14:AE:619:ILE:HG22  | 1.96                     | 0.47              |
| 14:AE:1108:GLN:HE21 | 14:AE:1123:ARG:HH12 | 1.62                     | 0.47              |
| 10:B:70:G:C2'       | 10:B:71:C:H5''      | 2.45                     | 0.47              |
| 16:C:12:ARG:CZ      | 16:C:13:PHE:CE1     | 2.97                     | 0.47              |
| 16:C:16:GLU:OE1     | 16:C:18:VAL:HB      | 2.15                     | 0.47              |
| 16:C:60:LYS:NZ      | 17:D:734:G:H2'      | 2.25                     | 0.47              |
| 16:C:60:LYS:HE3     | 17:D:735:C:H4'      | 1.97                     | 0.47              |
| 17:D:35:G:H2'       | 17:D:36:C:H6        | 1.79                     | 0.47              |
| 17:D:306:A:C5       | 17:D:307:C:C5       | 3.02                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 17:D:307:C:O2     | 17:D:307:C:H2'   | 2.15                     | 0.47              |
| 17:D:436:C:C2     | 17:D:437:U:C5    | 3.02                     | 0.47              |
| 17:D:611:C:C2     | 17:D:612:C:C5    | 3.02                     | 0.47              |
| 17:D:745:G:H2'    | 17:D:746:A:C8    | 2.50                     | 0.47              |
| 17:D:864:A:H5'    | 24:K:90:THR:O    | 2.14                     | 0.47              |
| 17:D:1189:U:OP1   | 32:S:98:LYS:NZ   | 2.48                     | 0.47              |
| 17:D:1382:C:N3    | 17:D:1383:C:C5   | 2.83                     | 0.47              |
| 19:F:19:PHE:HE2   | 30:Q:110:ILE:C   | 2.23                     | 0.47              |
| 19:F:64:ASN:HA    | 19:F:67:ARG:HD3  | 1.97                     | 0.47              |
| 21:H:70:VAL:HA    | 21:H:85:SER:HA   | 1.95                     | 0.47              |
| 21:H:277:GLY:CA   | 21:H:331:MET:CE  | 2.93                     | 0.47              |
| 22:I:132:ARG:CA   | 22:I:135:LYS:HE3 | 2.44                     | 0.47              |
| 23:J:62:ARG:HA    | 23:J:72:PHE:CZ   | 2.50                     | 0.47              |
| 29:P:13:PHE:CE1   | 29:P:67:ILE:HD11 | 2.50                     | 0.47              |
| 31:R:18:LYS:NZ    | 31:R:19:SER:O    | 2.47                     | 0.47              |
| 33:T:11:ILE:HG21  | 33:T:31:LEU:CD1  | 2.45                     | 0.47              |
| 35:V:27:ARG:HH12  | 35:V:42:THR:CB   | 2.26                     | 0.47              |
| 35:V:62:ARG:C     | 35:V:73:TRP:CE3  | 2.92                     | 0.47              |
| 38:Y:102:ARG:HH11 | 38:Y:141:ASP:CG  | 2.23                     | 0.47              |
| 40:a:257:C:O2     | 60:u:104:GLN:NE2 | 2.48                     | 0.47              |
| 40:a:592:A:C2     | 54:o:4:ILE:HD11  | 2.49                     | 0.47              |
| 40:a:921:C:C2     | 40:a:922:C:C5    | 3.03                     | 0.47              |
| 40:a:1429:G:H2'   | 40:a:1430:G:H8   | 1.79                     | 0.47              |
| 40:a:1790:C:O3'   | 40:a:1791:A:C8   | 2.68                     | 0.47              |
| 40:a:1844:C:C2    | 40:a:1845:G:C8   | 3.02                     | 0.47              |
| 40:a:2190:G:H2'   | 40:a:2191:A:C8   | 2.50                     | 0.47              |
| 40:a:2294:G:OP1   | 63:x:98:GLN:OE1  | 2.33                     | 0.47              |
| 40:a:2297:A:C6    | 40:a:2321:U:O4   | 2.68                     | 0.47              |
| 40:a:2299:U:H2'   | 40:a:2300:C:C6   | 2.49                     | 0.47              |
| 40:a:2300:C:H2'   | 40:a:2301:C:H6   | 1.79                     | 0.47              |
| 40:a:2314:A:P     | 53:n:88:LYS:NZ   | 2.87                     | 0.47              |
| 40:a:2520:C:C6    | 40:a:2567:G:H1'  | 2.50                     | 0.47              |
| 40:a:2702:G:C5    | 40:a:2703:C:C5   | 3.03                     | 0.47              |
| 40:a:2803:G:H2'   | 40:a:2804:U:C5   | 2.50                     | 0.47              |
| 44:e:20:ASN:HA    | 44:e:23:ARG:NE   | 2.30                     | 0.47              |
| 44:e:24:GLU:O     | 44:e:25:GLN:C    | 2.57                     | 0.47              |
| 47:h:181:MET:HE2  | 47:h:181:MET:CA  | 2.45                     | 0.47              |
| 51:l:42:GLY:HA3   | 51:l:92:HIS:HE1  | 1.80                     | 0.47              |
| 51:l:59:PRO:HB2   | 51:l:60:TRP:CE3  | 2.50                     | 0.47              |
| 51:l:112:LEU:HD21 | 51:l:186:VAL:HB  | 1.97                     | 0.47              |
| 51:l:148:ILE:CD1  | 51:l:187:VAL:HB  | 2.44                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 54:o:33:LEU:O      | 54:o:41:LYS:NZ      | 2.45                     | 0.47              |
| 58:s:72:LYS:HD3    | 58:s:74:TYR:CZ      | 2.43                     | 0.47              |
| 61:v:57:VAL:HG22   | 61:v:57:VAL:O       | 2.14                     | 0.47              |
| 63:x:90:VAL:HG13   | 63:x:115:LEU:HD11   | 1.96                     | 0.47              |
| 4:3:96:PHE:CE1     | 4:3:103:ILE:HG12    | 2.50                     | 0.47              |
| 5:4:21:ARG:HA      | 5:4:25:LYS:O        | 2.14                     | 0.47              |
| 6:5:10:DT:C4       | 11:AA:62:TYR:HE2    | 2.27                     | 0.47              |
| 6:5:10:DT:C4'      | 11:AA:62:TYR:OH     | 2.61                     | 0.47              |
| 9:9:18:VAL:CG1     | 9:9:71:CYS:HB2      | 2.45                     | 0.47              |
| 9:9:40:GLU:CD      | 9:9:54:VAL:HG11     | 2.39                     | 0.47              |
| 10:A:52:G:C6       | 10:A:63:G:O6        | 2.68                     | 0.47              |
| 14:AE:86:GLU:N     | 14:AE:86:GLU:CD     | 2.73                     | 0.47              |
| 14:AE:1350:ASN:HA  | 14:AE:1353:VAL:HG12 | 1.97                     | 0.47              |
| 10:B:52:G:C6       | 10:B:63:G:O6        | 2.68                     | 0.47              |
| 17:D:22:G:C5       | 17:D:23:C:C5        | 3.03                     | 0.47              |
| 17:D:375:U:H1'     | 34:U:28:ARG:HH22    | 1.79                     | 0.47              |
| 20:G:110:SER:HA    | 20:G:113:ARG:HH21   | 1.79                     | 0.47              |
| 22:I:22:TRP:CZ2    | 22:I:32:ASN:HB2     | 2.50                     | 0.47              |
| 26:M:111:ARG:O     | 26:M:119:ARG:CZ     | 2.63                     | 0.47              |
| 29:P:10:LEU:C      | 29:P:11:LYS:HD3     | 2.40                     | 0.47              |
| 33:T:48:LYS:O      | 33:T:50:HIS:N       | 2.48                     | 0.47              |
| 40:a:879:G:H2'     | 40:a:880:G:O4'      | 2.14                     | 0.47              |
| 40:a:880:G:C2      | 40:a:881:G:C8       | 3.02                     | 0.47              |
| 40:a:2294:G:OP1    | 63:x:10:ARG:HD3     | 2.15                     | 0.47              |
| 40:a:2351:G:O6     | 54:o:39:LYS:NZ      | 2.48                     | 0.47              |
| 40:a:2517:C:O2     | 40:a:2542:A:N6      | 2.48                     | 0.47              |
| 49:j:9:VAL:O       | 49:j:197:THR:HG23   | 2.15                     | 0.47              |
| 51:l:6:LYS:HZ1     | 51:l:119:ILE:C      | 2.23                     | 0.47              |
| 54:o:62:LEU:HG     | 54:o:65:ALA:HA      | 1.95                     | 0.47              |
| 55:p:52:PHE:CZ     | 55:p:72:LEU:HD22    | 2.50                     | 0.47              |
| 61:v:30:SER:N      | 61:v:104:GLU:OE2    | 2.48                     | 0.47              |
| 63:x:83:LEU:HD23   | 63:x:88:LYS:HE3     | 1.97                     | 0.47              |
| 1:0:4:VAL:HG23     | 1:0:39:LEU:HB2      | 1.97                     | 0.47              |
| 9:9:69:PHE:C       | 9:9:72:LEU:HD11     | 2.40                     | 0.47              |
| 10:A:70:G:C2'      | 10:A:71:C:H5''      | 2.45                     | 0.47              |
| 14:AE:66:LYS:HB2   | 14:AE:69:GLU:HB3    | 1.96                     | 0.47              |
| 14:AE:319:SER:HA   | 14:AE:320:ASN:HA    | 1.73                     | 0.47              |
| 14:AE:797:THR:HG22 | 14:AE:924:GLY:HA3   | 1.97                     | 0.47              |
| 10:B:47:U:H2'      | 10:B:48:C:H4'       | 1.97                     | 0.47              |
| 10:B:48:C:C2'      | 10:B:49:G:OP2       | 2.62                     | 0.47              |
| 10:B:68:C:H3'      | 10:B:69:C:H5''      | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:D:13:U:C4      | 17:D:21:G:C2      | 3.03                     | 0.47              |
| 20:G:19:GLN:OE1   | 20:G:21:ARG:CG    | 2.63                     | 0.47              |
| 21:H:37:LEU:HD11  | 21:H:47:ALA:HA    | 1.96                     | 0.47              |
| 22:I:107:ARG:HB3  | 22:I:108:LYS:HD2  | 1.97                     | 0.47              |
| 23:J:41:HIS:ND1   | 23:J:44:ARG:NH1   | 2.63                     | 0.47              |
| 24:K:165:LEU:HD12 | 27:N:114:ARG:NH1  | 2.30                     | 0.47              |
| 27:N:3:MET:O      | 27:N:3:MET:HE3    | 2.14                     | 0.47              |
| 28:O:127:PHE:CD1  | 28:O:128:SER:N    | 2.83                     | 0.47              |
| 32:S:63:ARG:NH2   | 32:S:70:PRO:HD3   | 2.30                     | 0.47              |
| 38:Y:96:LYS:HD2   | 38:Y:136:GLY:O    | 2.15                     | 0.47              |
| 40:a:1200:C:C2    | 40:a:1201:U:C5    | 3.03                     | 0.47              |
| 40:a:1467:U:C4    | 40:a:1546:G:C2    | 3.03                     | 0.47              |
| 40:a:1936:A:N7    | 40:a:1945:G:C8    | 2.83                     | 0.47              |
| 40:a:2200:C:OP2   | 42:c:37:ARG:NH2   | 2.48                     | 0.47              |
| 40:a:2250:G:OP1   | 61:v:84:LYS:NZ    | 2.48                     | 0.47              |
| 40:a:2513:A:H2'   | 40:a:2514:U:C6    | 2.50                     | 0.47              |
| 40:a:2700:A:H2'   | 40:a:2701:U:C6    | 2.50                     | 0.47              |
| 46:g:18:CYS:HB2   | 46:g:40:CYS:HB3   | 1.96                     | 0.47              |
| 57:r:58:LEU:O     | 57:r:61:VAL:HG22  | 2.14                     | 0.47              |
| 60:u:19:LEU:CD2   | 60:u:27:LEU:HD12  | 2.45                     | 0.47              |
| 61:v:31:PHE:O     | 61:v:104:GLU:OE1  | 2.33                     | 0.47              |
| 1:0:4:VAL:CG2     | 1:0:40:MET:HB3    | 2.45                     | 0.47              |
| 2:1:105:VAL:HG13  | 2:1:105:VAL:O     | 2.14                     | 0.47              |
| 3:2:56:GLU:OE2    | 3:2:88:LYS:CA     | 2.61                     | 0.47              |
| 9:9:3:LEU:O       | 9:9:4:ASN:OD1     | 2.33                     | 0.47              |
| 10:A:47:U:H2'     | 10:A:48:C:H4'     | 1.97                     | 0.47              |
| 10:A:48:C:C2'     | 10:A:49:G:OP2     | 2.62                     | 0.47              |
| 11:AA:318:SER:OG  | 11:AA:320:ASP:OD1 | 2.31                     | 0.47              |
| 11:AA:1311:GLY:O  | 15:AF:31:GLN:NE2  | 2.47                     | 0.47              |
| 17:D:339:C:H2'    | 17:D:340:U:C6     | 2.50                     | 0.47              |
| 17:D:1363:A:C5    | 17:D:1365:G:C6    | 3.03                     | 0.47              |
| 17:D:1368:A:OP1   | 28:O:113:ARG:NH2  | 2.48                     | 0.47              |
| 20:G:18:HIS:CE1   | 20:G:205:ASP:OD1  | 2.68                     | 0.47              |
| 23:J:74:ASN:CA    | 23:J:77:LYS:HZ3   | 2.28                     | 0.47              |
| 24:K:156:LYS:HE3  | 27:N:71:VAL:CG1   | 2.42                     | 0.47              |
| 26:M:116:MET:HA   | 26:M:119:ARG:HD3  | 1.97                     | 0.47              |
| 28:O:63:LEU:HD13  | 28:O:65:ILE:HD11  | 1.97                     | 0.47              |
| 29:P:13:PHE:CZ    | 29:P:67:ILE:HD11  | 2.50                     | 0.47              |
| 30:Q:20:VAL:HB    | 30:Q:35:THR:CG2   | 2.45                     | 0.47              |
| 31:R:74:LEU:HD11  | 31:R:80:ILE:HG13  | 1.96                     | 0.47              |
| 36:W:63:THR:HG22  | 36:W:64:ASP:N     | 2.30                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:a:451:U:C5'    | 51:l:47:LYS:HZ3   | 2.28                     | 0.47              |
| 40:a:909:A:H2'    | 40:a:912:C:H5     | 1.80                     | 0.47              |
| 40:a:1441:G:H2'   | 40:a:1442:U:C6    | 2.50                     | 0.47              |
| 40:a:1656:C:P     | 49:j:141:ARG:HD2  | 2.55                     | 0.47              |
| 40:a:1790:C:H2'   | 40:a:1791:A:N7    | 2.29                     | 0.47              |
| 40:a:1794:A:H2'   | 40:a:1795:C:C6    | 2.50                     | 0.47              |
| 40:a:2013:A:C2    | 40:a:2613:U:O4    | 2.68                     | 0.47              |
| 40:a:2766:A:C5    | 40:a:2767:C:C5    | 3.03                     | 0.47              |
| 40:a:2840:C:C2    | 40:a:2841:C:C5    | 3.03                     | 0.47              |
| 43:d:42:C:C5      | 53:n:66:LEU:HD12  | 2.49                     | 0.47              |
| 53:n:12:VAL:O     | 53:n:16:LEU:HG    | 2.14                     | 0.47              |
| 61:v:41:LEU:HG    | 61:v:96:ILE:CG1   | 2.45                     | 0.47              |
| 62:w:24:MET:HG3   | 62:w:44:LEU:HD12  | 1.97                     | 0.47              |
| 62:w:44:LEU:C     | 62:w:44:LEU:HD23  | 2.40                     | 0.47              |
| 65:z:69:ALA:HA    | 65:z:106:PHE:HZ   | 1.80                     | 0.47              |
| 12:AB:6:LEU:CD1   | 14:AE:291:ILE:CD1 | 2.84                     | 0.46              |
| 16:C:12:ARG:NH1   | 16:C:13:PHE:CE1   | 2.84                     | 0.46              |
| 17:D:126:G:OP1    | 17:D:605:U:O2'    | 2.19                     | 0.46              |
| 17:D:1238:A:H2    | 17:D:1241:G:N3    | 2.13                     | 0.46              |
| 18:E:9:LYS:O      | 18:E:12:ILE:HG12  | 2.14                     | 0.46              |
| 20:G:197:ASP:OD2  | 20:G:198:PHE:CE2  | 2.68                     | 0.46              |
| 24:K:96:MET:HG2   | 24:K:125:ALA:HB2  | 1.97                     | 0.46              |
| 25:L:17:GLN:C     | 25:L:21:MET:HE1   | 2.40                     | 0.46              |
| 26:M:18:PHE:CD2   | 26:M:59:LEU:HD21  | 2.46                     | 0.46              |
| 28:O:89:GLU:O     | 28:O:92:GLU:OE1   | 2.32                     | 0.46              |
| 30:Q:116:ILE:HG13 | 30:Q:116:ILE:O    | 2.14                     | 0.46              |
| 32:S:79:LEU:HB2   | 32:S:84:VAL:CG2   | 2.45                     | 0.46              |
| 33:T:71:LYS:HZ3   | 33:T:78:TYR:HD2   | 1.61                     | 0.46              |
| 40:a:104:A:C5     | 40:a:105:C:C5     | 3.02                     | 0.46              |
| 40:a:404:A:H4'    | 40:a:405:U:O5'    | 2.15                     | 0.46              |
| 40:a:858:G:P      | 41:b:78:LYS:HZ1   | 2.36                     | 0.46              |
| 40:a:871:U:H2'    | 40:a:872:U:H6     | 1.78                     | 0.46              |
| 40:a:872:U:H2'    | 40:a:873:C:C6     | 2.50                     | 0.46              |
| 40:a:1278:C:H2'   | 40:a:1279:G:H8    | 1.80                     | 0.46              |
| 40:a:2197:U:C5    | 40:a:2224:G:C6    | 3.03                     | 0.46              |
| 40:a:2345:G:C5    | 40:a:2347:C:C5    | 3.03                     | 0.46              |
| 41:b:53:CYS:SG    | 41:b:57:HIS:HA    | 2.55                     | 0.46              |
| 65:z:108:ALA:O    | 65:z:112:LYS:HG2  | 2.15                     | 0.46              |
| 3:2:18:GLU:O      | 3:2:22:THR:HG23   | 2.15                     | 0.46              |
| 4:3:47:LYS:NZ     | 40:a:482:A:O5'    | 2.48                     | 0.46              |
| 5:4:53:LYS:HB3    | 5:4:55:GLU:OE1    | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:4:53:LYS:O      | 5:4:56:PHE:HD2    | 1.97                     | 0.46              |
| 14:AE:516:ASP:OD1 | 14:AE:516:ASP:N   | 2.47                     | 0.46              |
| 16:C:21:ILE:CD1   | 16:C:54:GLN:NE2   | 2.78                     | 0.46              |
| 17:D:821:G:H2'    | 17:D:822:U:H6     | 1.80                     | 0.46              |
| 19:F:37:PHE:HA    | 30:Q:123:PRO:HB2  | 1.97                     | 0.46              |
| 21:H:277:GLY:HA2  | 21:H:331:MET:HE3  | 1.97                     | 0.46              |
| 22:I:134:MET:HE2  | 22:I:168:TYR:CB   | 2.46                     | 0.46              |
| 25:L:43:GLY:HA2   | 25:L:58:HIS:CE1   | 2.51                     | 0.46              |
| 26:M:74:GLU:CG    | 26:M:91:VAL:CG1   | 2.94                     | 0.46              |
| 27:N:112:THR:HG23 | 27:N:115:ALA:H    | 1.80                     | 0.46              |
| 36:W:77:THR:OG1   | 36:W:78:ARG:HD2   | 2.15                     | 0.46              |
| 40:a:57:C:C2      | 40:a:58:G:C8      | 3.04                     | 0.46              |
| 40:a:753:A:C6     | 40:a:754:U:C5     | 3.04                     | 0.46              |
| 40:a:1006:C:C2    | 40:a:1138:G:N2    | 2.83                     | 0.46              |
| 40:a:1405:U:H2'   | 40:a:1406:U:C5    | 2.49                     | 0.46              |
| 40:a:1786:A:H1'   | 40:a:1938:A:N6    | 2.30                     | 0.46              |
| 40:a:2646:C:O5'   | 40:a:2646:C:H6    | 1.98                     | 0.46              |
| 55:p:8:PRO:C      | 55:p:69:ARG:HH21  | 2.22                     | 0.46              |
| 56:q:2:LYS:HE2    | 56:q:35:GLN:HG3   | 1.97                     | 0.46              |
| 58:s:56:VAL:O     | 58:s:124:VAL:HA   | 2.14                     | 0.46              |
| 59:t:50:GLY:O     | 59:t:53:LYS:NZ    | 2.47                     | 0.46              |
| 61:v:111:GLU:O    | 61:v:112:LEU:C    | 2.57                     | 0.46              |
| 5:4:23:ALA:O      | 5:4:24:ASN:OD1    | 2.33                     | 0.46              |
| 8:7:7:U:C6        | 8:7:7:U:C3'       | 2.97                     | 0.46              |
| 9:9:38:MET:HA     | 9:9:41:LEU:HD12   | 1.96                     | 0.46              |
| 14:AE:287:ALA:HB3 | 14:AE:292:VAL:CG2 | 2.46                     | 0.46              |
| 10:B:75:C:O2'     | 10:B:76:A:N7      | 2.48                     | 0.46              |
| 16:C:31:ASN:OD1   | 21:H:268:VAL:HG12 | 2.15                     | 0.46              |
| 17:D:35:G:N3      | 31:R:115:SER:OG   | 2.47                     | 0.46              |
| 17:D:739:C:O2'    | 33:T:42:HIS:CE1   | 2.68                     | 0.46              |
| 17:D:983:A:H5'    | 17:D:984:C:OP2    | 2.15                     | 0.46              |
| 17:D:1328:C:O3'   | 37:X:28:THR:HB    | 2.16                     | 0.46              |
| 22:I:134:MET:HE1  | 22:I:167:TRP:CA   | 2.43                     | 0.46              |
| 26:M:69:VAL:HA    | 26:M:138:ARG:HD3  | 1.97                     | 0.46              |
| 26:M:95:ARG:CZ    | 26:M:99:LEU:HD21  | 2.45                     | 0.46              |
| 28:O:7:TYR:O      | 28:O:89:GLU:CD    | 2.58                     | 0.46              |
| 37:X:3:ARG:HB3    | 46:g:35:ASP:OD2   | 2.15                     | 0.46              |
| 38:Y:37:PHE:HZ    | 38:Y:56:VAL:HG11  | 1.79                     | 0.46              |
| 40:a:396:G:C6     | 40:a:397:U:C4     | 3.04                     | 0.46              |
| 40:a:626:A:C2     | 60:u:78:ARG:CZ    | 2.98                     | 0.46              |
| 40:a:666:A:H4'    | 60:u:48:ARG:HD2   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:a:1068:G:O6    | 40:a:1069:A:N6    | 2.48                     | 0.46              |
| 40:a:2700:A:H2'   | 40:a:2701:U:H6    | 1.80                     | 0.46              |
| 40:a:2784:U:H2'   | 40:a:2785:C:H6    | 1.80                     | 0.46              |
| 41:b:51:VAL:HG12  | 41:b:59:LEU:HD12  | 1.96                     | 0.46              |
| 43:d:82:U:O2'     | 45:f:53:PHE:HE2   | 1.98                     | 0.46              |
| 48:i:28:LEU:HB2   | 48:i:37:LYS:HE3   | 1.97                     | 0.46              |
| 51:l:195:GLN:CA   | 51:l:198:GLU:OE1  | 2.64                     | 0.46              |
| 58:s:136:GLN:N    | 58:s:137:PRO:CD   | 2.78                     | 0.46              |
| 60:u:110:VAL:HG23 | 60:u:125:LEU:HD12 | 1.97                     | 0.46              |
| 3:2:3:ARG:CZ      | 3:2:5:GLU:OE1     | 2.64                     | 0.46              |
| 5:4:53:LYS:HD2    | 5:4:56:PHE:HE2    | 1.77                     | 0.46              |
| 9:9:25:ALA:HB3    | 9:9:99:PHE:CE2    | 2.51                     | 0.46              |
| 9:9:60:LEU:O      | 9:9:64:VAL:HB     | 2.15                     | 0.46              |
| 10:A:19:G:O6      | 40:a:2112:G:O5'   | 2.34                     | 0.46              |
| 12:AB:123:PHE:CZ  | 29:P:82:LYS:CA    | 2.72                     | 0.46              |
| 12:AB:126:PHE:HE1 | 14:AE:87:LYS:HG2  | 1.81                     | 0.46              |
| 14:AE:287:ALA:CB  | 14:AE:292:VAL:CG2 | 2.93                     | 0.46              |
| 17:D:216:U:H2'    | 17:D:217:C:C6     | 2.50                     | 0.46              |
| 17:D:610:U:N3     | 17:D:611:C:C5     | 2.83                     | 0.46              |
| 17:D:737:C:C2     | 17:D:738:C:C5     | 3.03                     | 0.46              |
| 20:G:207:ILE:HG23 | 20:G:208:ARG:N    | 2.30                     | 0.46              |
| 21:H:302:GLY:HA3  | 21:H:344:LEU:HD13 | 1.96                     | 0.46              |
| 26:M:69:VAL:HG23  | 26:M:100:ALA:HB1  | 1.97                     | 0.46              |
| 36:W:9:PRO:HB3    | 46:g:64:PHE:CZ    | 2.51                     | 0.46              |
| 40:a:136:G:C6     | 40:a:144:A:C6     | 3.04                     | 0.46              |
| 40:a:391:A:C5     | 40:a:392:U:C5     | 3.04                     | 0.46              |
| 40:a:1477:A:N6    | 40:a:1514:G:O2'   | 2.45                     | 0.46              |
| 40:a:2236:U:H2'   | 40:a:2237:G:O4'   | 2.15                     | 0.46              |
| 40:a:2314:A:O2'   | 53:n:155:THR:HG21 | 2.15                     | 0.46              |
| 40:a:2393:U:C5'   | 54:o:30:ARG:NH1   | 2.76                     | 0.46              |
| 40:a:2683:C:H4'   | 49:j:13:ARG:NH1   | 2.31                     | 0.46              |
| 40:a:2748:A:C2    | 40:a:2757:A:C5    | 3.03                     | 0.46              |
| 42:c:71:LEU:O     | 42:c:76:GLU:HG3   | 2.16                     | 0.46              |
| 47:h:2:ALA:N      | 47:h:20:VAL:O     | 2.49                     | 0.46              |
| 49:j:1:MET:O      | 49:j:204:LYS:HD2  | 2.15                     | 0.46              |
| 50:k:34:LEU:HB2   | 50:k:51:GLU:OE2   | 2.16                     | 0.46              |
| 57:r:18:GLN:OE1   | 57:r:39:ALA:HB1   | 2.15                     | 0.46              |
| 65:z:69:ALA:O     | 65:z:74:ILE:HG22  | 2.15                     | 0.46              |
| 65:z:113:ALA:O    | 65:z:117:LEU:HD13 | 2.15                     | 0.46              |
| 2:1:50:VAL:HG12   | 2:1:105:VAL:CG1   | 2.45                     | 0.46              |
| 6:5:10:DT:OP1     | 11:AA:476:LYS:HD2 | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:7:29:U:H3'       | 8:7:29:U:H6        | 1.80                     | 0.46              |
| 10:B:24:U:H2'      | 10:B:25:C:C6       | 2.51                     | 0.46              |
| 17:D:611:C:C2      | 17:D:612:C:C6      | 3.04                     | 0.46              |
| 17:D:1055:A:H1'    | 22:I:156:ARG:NH2   | 2.31                     | 0.46              |
| 17:D:1109:C:C2     | 17:D:1110:A:C8     | 3.04                     | 0.46              |
| 17:D:1458:G:H5''   | 18:E:26:SER:OG     | 2.14                     | 0.46              |
| 21:H:270:ILE:HG23  | 21:H:270:ILE:O     | 2.15                     | 0.46              |
| 21:H:287:LEU:HG    | 21:H:292:CYS:HA    | 1.98                     | 0.46              |
| 24:K:143:GLY:O     | 24:K:146:ASN:OD1   | 2.34                     | 0.46              |
| 25:L:99:ALA:HB3    | 25:L:104:LYS:HZ1   | 1.80                     | 0.46              |
| 28:O:58:VAL:HG23   | 28:O:59:GLU:N      | 2.31                     | 0.46              |
| 32:S:6:MET:HE3     | 32:S:63:ARG:NH1    | 2.31                     | 0.46              |
| 40:a:6:A:H5'       | 58:s:131:ASN:OD1   | 2.15                     | 0.46              |
| 40:a:15:G:O2'      | 48:i:15:MET:HE2    | 2.15                     | 0.46              |
| 40:a:581:C:H2'     | 40:a:582:A:C8      | 2.50                     | 0.46              |
| 40:a:832:U:H2'     | 40:a:833:A:C8      | 2.50                     | 0.46              |
| 40:a:1223:G:N2     | 40:a:1226:A:OP2    | 2.43                     | 0.46              |
| 40:a:1433:A:H2'    | 40:a:1434:A:C1'    | 2.46                     | 0.46              |
| 40:a:1598:A:C4     | 40:a:1599:U:C6     | 3.03                     | 0.46              |
| 40:a:1665:A:O3'    | 59:t:66:LYS:NZ     | 2.44                     | 0.46              |
| 40:a:1791:A:C2     | 40:a:1829:A:H4'    | 2.49                     | 0.46              |
| 40:a:2093:G:O2'    | 40:a:2198:A:N1     | 2.41                     | 0.46              |
| 40:a:2362:C:OP2    | 54:o:40:ARG:CZ     | 2.63                     | 0.46              |
| 46:g:8:LYS:NZ      | 46:g:10:GLU:HB2    | 2.31                     | 0.46              |
| 46:g:16:CYS:CB     | 46:g:37:CYS:CB     | 2.90                     | 0.46              |
| 46:g:56:ARG:HH21   | 46:g:59:ARG:HH21   | 1.62                     | 0.46              |
| 47:h:108:LYS:HZ3   | 47:h:194:GLU:N     | 2.13                     | 0.46              |
| 48:i:4:GLN:OE1     | 48:i:7:LYS:HA      | 2.16                     | 0.46              |
| 51:l:1:MET:CE      | 51:l:20:GLY:N      | 2.79                     | 0.46              |
| 55:p:155:GLU:O     | 55:p:159:GLY:HA2   | 2.15                     | 0.46              |
| 9:9:43:LYS:HE3     | 9:9:102:ALA:HB2    | 1.97                     | 0.46              |
| 10:A:24:U:H2'      | 10:A:25:C:C6       | 2.51                     | 0.46              |
| 11:AA:103:VAL:HG12 | 11:AA:117:ILE:HG22 | 1.97                     | 0.46              |
| 13:AD:212:ASP:OD1  | 13:AD:212:ASP:N    | 2.48                     | 0.46              |
| 14:AE:79:LYS:CB    | 14:AE:81:ARG:NH1   | 2.73                     | 0.46              |
| 14:AE:1037:PHE:HB3 | 14:AE:1040:MET:HB2 | 1.97                     | 0.46              |
| 10:B:50:U:H2'      | 10:B:51:C:C6       | 2.51                     | 0.46              |
| 10:B:65:C:C2'      | 10:B:66:C:H5'      | 2.44                     | 0.46              |
| 16:C:34:THR:HB     | 16:C:38:LYS:H      | 1.81                     | 0.46              |
| 16:C:63:ARG:HB3    | 16:C:70:TYR:CE1    | 2.51                     | 0.46              |
| 17:D:110:C:O4'     | 34:U:25:ARG:NH2    | 2.49                     | 0.46              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 17:D:1435:G:H2'  | 17:D:1436:U:C6     | 2.51                     | 0.46              |
| 19:F:12:PHE:CD1  | 30:Q:101:ASN:ND2   | 2.84                     | 0.46              |
| 21:H:304:VAL:O   | 21:H:304:VAL:CG1   | 2.63                     | 0.46              |
| 22:I:49:LYS:HZ3  | 22:I:75:ILE:HD11   | 1.81                     | 0.46              |
| 22:I:181:ASP:HB2 | 22:I:207:ILE:HD11  | 1.97                     | 0.46              |
| 27:N:6:PRO:O     | 27:N:33:LYS:NZ     | 2.48                     | 0.46              |
| 33:T:47:LYS:HD3  | 33:T:47:LYS:N      | 2.30                     | 0.46              |
| 38:Y:102:ARG:NE  | 38:Y:139:VAL:CG2   | 2.78                     | 0.46              |
| 40:a:78:U:OP1    | 44:e:4:LYS:CE      | 2.63                     | 0.46              |
| 40:a:374:A:C2    | 40:a:375:G:H1'     | 2.51                     | 0.46              |
| 40:a:1069:A:O2'  | 40:a:1073:A:N6     | 2.38                     | 0.46              |
| 40:a:2454:G:C6   | 40:a:2499:C:N4     | 2.83                     | 0.46              |
| 40:a:2725:A:C4   | 40:a:2727:A:N7     | 2.83                     | 0.46              |
| 40:a:2743:U:O2'  | 55:p:153:ARG:NH1   | 2.49                     | 0.46              |
| 42:c:76:GLU:OE1  | 42:c:77:LYS:O      | 2.34                     | 0.46              |
| 47:h:138:GLY:H   | 47:h:164:ILE:HG23  | 1.79                     | 0.46              |
| 53:n:171:ALA:O   | 53:n:174:ASP:N     | 2.47                     | 0.46              |
| 58:s:55:ILE:HG13 | 58:s:123:LYS:CE    | 2.46                     | 0.46              |
| 59:t:8:LEU:N     | 59:t:8:LEU:HD12    | 2.30                     | 0.46              |
| 59:t:42:THR:C    | 59:t:44:LYS:HZ2    | 2.15                     | 0.46              |
| 1:0:71:LYS:HE2   | 1:0:90:ARG:HD2     | 1.97                     | 0.46              |
| 9:9:59:LEU:HB2   | 9:9:62:ARG:CG      | 2.45                     | 0.46              |
| 12:AB:140:MET:O  | 12:AB:151:LYS:O    | 2.34                     | 0.46              |
| 13:AD:185:TYR:HA | 13:AD:202:VAL:O    | 2.16                     | 0.46              |
| 14:AE:218:THR:HA | 14:AE:221:ILE:HG22 | 1.96                     | 0.46              |
| 17:D:197:A:C6    | 17:D:221:C:H4'     | 2.50                     | 0.46              |
| 17:D:771:G:C6    | 17:D:809:G:C6      | 3.03                     | 0.46              |
| 17:D:826:C:O2    | 27:N:16:ASN:ND2    | 2.49                     | 0.46              |
| 17:D:1226:C:H4'  | 17:D:1227:A:OP1    | 2.16                     | 0.46              |
| 18:E:82:GLN:HA   | 18:E:85:LYS:NZ     | 2.31                     | 0.46              |
| 22:I:58:GLU:OE2  | 29:P:94:ALA:HB1    | 2.16                     | 0.46              |
| 22:I:85:GLU:O    | 22:I:89:LYS:CE     | 2.64                     | 0.46              |
| 25:L:96:VAL:O    | 25:L:96:VAL:HG23   | 2.16                     | 0.46              |
| 27:N:114:ARG:HD2 | 27:N:114:ARG:C     | 2.41                     | 0.46              |
| 31:R:2:ALA:CA    | 31:R:7:LEU:HD11    | 2.45                     | 0.46              |
| 33:T:15:PHE:CD2  | 33:T:30:ALA:HB2    | 2.49                     | 0.46              |
| 38:Y:106:GLN:OE1 | 38:Y:125:THR:HG21  | 2.15                     | 0.46              |
| 40:a:182:A:H2'   | 40:a:183:C:H6      | 1.81                     | 0.46              |
| 40:a:584:C:N4    | 40:a:585:G:C6      | 2.83                     | 0.46              |
| 40:a:1585:C:H2'  | 40:a:1586:A:O4'    | 2.15                     | 0.46              |
| 40:a:1796:U:H2'  | 40:a:1797:G:C8     | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:a:2616:C:N3    | 40:a:2617:U:C5    | 2.83                     | 0.46              |
| 43:d:44:G:H3'     | 53:n:92:ARG:HH22  | 1.81                     | 0.46              |
| 44:e:12:GLU:CG    | 44:e:13:GLU:N     | 2.78                     | 0.46              |
| 44:e:12:GLU:HG2   | 44:e:13:GLU:H     | 1.80                     | 0.46              |
| 51:l:35:TYR:CD2   | 51:l:178:VAL:HG11 | 2.51                     | 0.46              |
| 51:l:175:ILE:HG21 | 51:l:180:LEU:HD11 | 1.97                     | 0.46              |
| 58:s:25:LEU:HD11  | 58:s:101:ILE:HD13 | 1.97                     | 0.46              |
| 58:s:123:LYS:HD2  | 58:s:132:HIS:CD2  | 2.50                     | 0.46              |
| 3:2:57:VAL:HG12   | 3:2:86:THR:OG1    | 2.15                     | 0.46              |
| 5:4:80:HIS:CE1    | 5:4:83:LYS:HZ3    | 2.33                     | 0.46              |
| 5:4:80:HIS:CD2    | 5:4:83:LYS:HZ3    | 2.32                     | 0.46              |
| 10:A:32:C:C2'     | 10:A:33:U:H5'     | 2.46                     | 0.46              |
| 11:AA:207:THR:OG1 | 11:AA:354:ASP:OD2 | 2.32                     | 0.46              |
| 12:AB:119:THR:HB  | 12:AB:125:GLY:HA2 | 1.97                     | 0.46              |
| 10:B:75:C:P       | 40:a:2602:A:H2'   | 2.55                     | 0.46              |
| 17:D:1324:A:H2'   | 17:D:1325:C:C6    | 2.51                     | 0.46              |
| 19:F:16:LEU:HD12  | 30:Q:98:ARG:HH21  | 1.81                     | 0.46              |
| 24:K:16:ILE:HD11  | 24:K:38:VAL:CG1   | 2.46                     | 0.46              |
| 26:M:17:LYS:HZ2   | 26:M:18:PHE:HD1   | 1.60                     | 0.46              |
| 31:R:5:ASN:HB3    | 31:R:9:ARG:HH22   | 1.80                     | 0.46              |
| 33:T:3:LEU:HD23   | 33:T:4:SER:O      | 2.15                     | 0.46              |
| 40:a:609:A:H3'    | 40:a:610:C:H6     | 1.80                     | 0.46              |
| 40:a:858:G:OP2    | 41:b:78:LYS:NZ    | 2.34                     | 0.46              |
| 40:a:1688:U:O2'   | 40:a:1700:A:N7    | 2.44                     | 0.46              |
| 40:a:1803:A:O2'   | 47:h:257:THR:HG21 | 2.16                     | 0.46              |
| 40:a:2357:G:P     | 41:b:20:ARG:CZ    | 3.04                     | 0.46              |
| 43:d:83:G:H1'     | 45:f:53:PHE:CE1   | 2.51                     | 0.46              |
| 44:e:10:SER:OG    | 44:e:12:GLU:HG2   | 2.15                     | 0.46              |
| 46:g:47:LYS:CD    | 53:n:178:ARG:HH22 | 2.29                     | 0.46              |
| 47:h:52:ARG:NE    | 47:h:53:HIS:CE1   | 2.83                     | 0.46              |
| 48:i:40:ARG:HH12  | 48:i:41:HIS:CD2   | 2.34                     | 0.46              |
| 51:l:130:LYS:HB2  | 51:l:133:LEU:HD12 | 1.97                     | 0.46              |
| 55:p:69:ARG:NH1   | 55:p:73:ASN:CG    | 2.74                     | 0.46              |
| 57:r:72:ILE:HG22  | 57:r:72:ILE:O     | 2.16                     | 0.46              |
| 58:s:17:VAL:HG23  | 58:s:137:PRO:HB2  | 1.98                     | 0.46              |
| 1:0:58:VAL:HG13   | 1:0:60:LYS:HZ3    | 1.79                     | 0.46              |
| 3:2:3:ARG:HH22    | 3:2:4:GLU:HB2     | 1.81                     | 0.46              |
| 8:7:32:U:H4'      | 14:AE:322:ARG:CZ  | 2.46                     | 0.46              |
| 9:9:24:SER:HB3    | 9:9:116:GLU:HG3   | 1.94                     | 0.46              |
| 10:A:50:U:H2'     | 10:A:51:C:C6      | 2.51                     | 0.46              |
| 11:AA:230:PHE:HB2 | 11:AA:333:ILE:HB  | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AA:800:MET:HB2  | 11:AA:800:MET:HE3  | 1.69                     | 0.46              |
| 12:AB:116:VAL:HG23 | 12:AB:130:PHE:CZ   | 2.50                     | 0.46              |
| 12:AB:147:ASN:OD1  | 29:P:101:SER:HA    | 2.16                     | 0.46              |
| 13:AD:59:VAL:HG22  | 13:AD:144:ILE:HA   | 1.97                     | 0.46              |
| 14:AE:1341:ARG:NH1 | 14:AE:1343:GLU:OE2 | 2.49                     | 0.46              |
| 15:AF:25:ARG:NH1   | 15:AF:61:ASN:OD1   | 2.49                     | 0.46              |
| 16:C:33:ILE:O      | 21:H:338:GLU:CG    | 2.64                     | 0.46              |
| 16:C:65:LEU:HG     | 16:C:65:LEU:O      | 2.16                     | 0.46              |
| 17:D:371:A:H2'     | 17:D:372:C:O4'     | 2.15                     | 0.46              |
| 17:D:642:A:H2'     | 17:D:643:C:H6      | 1.80                     | 0.46              |
| 17:D:827:U:O4      | 17:D:872:A:C2      | 2.69                     | 0.46              |
| 17:D:915:A:C5      | 17:D:916:U:C6      | 3.04                     | 0.46              |
| 17:D:915:A:C6      | 17:D:916:U:C5      | 3.04                     | 0.46              |
| 17:D:928:G:H2'     | 17:D:929:G:H8      | 1.81                     | 0.46              |
| 17:D:1512:U:H2'    | 17:D:1513:A:C8     | 2.51                     | 0.46              |
| 19:F:12:PHE:CE1    | 30:Q:107:ILE:CG2   | 2.98                     | 0.46              |
| 21:H:303:LEU:C     | 21:H:305:HIS:N     | 2.73                     | 0.46              |
| 23:J:95:GLU:HG3    | 23:J:186:PRO:HG3   | 1.98                     | 0.46              |
| 24:K:150:PRO:O     | 24:K:153:VAL:HG22  | 2.16                     | 0.46              |
| 25:L:29:ILE:HG21   | 25:L:64:VAL:HG13   | 1.97                     | 0.46              |
| 25:L:47:LEU:HD13   | 25:L:51:ILE:HG12   | 1.98                     | 0.46              |
| 29:P:10:LEU:HD22   | 29:P:22:THR:HG22   | 1.98                     | 0.46              |
| 33:T:75:VAL:HG13   | 33:T:76:ALA:N      | 2.31                     | 0.46              |
| 35:V:7:THR:CG2     | 35:V:60:GLU:OE2    | 2.63                     | 0.46              |
| 35:V:61:ILE:C      | 35:V:73:TRP:HZ3    | 2.23                     | 0.46              |
| 36:W:32:ARG:NH2    | 36:W:34:TRP:CZ3    | 2.84                     | 0.46              |
| 36:W:32:ARG:NH2    | 36:W:34:TRP:HZ3    | 2.14                     | 0.46              |
| 38:Y:59:THR:O      | 38:Y:66:PHE:HB2    | 2.16                     | 0.46              |
| 40:a:644:A:H2'     | 40:a:645:C:O4'     | 2.15                     | 0.46              |
| 40:a:985:C:N3      | 40:a:986:C:C5      | 2.84                     | 0.46              |
| 40:a:1406:U:O2'    | 40:a:1407:G:P      | 2.74                     | 0.46              |
| 40:a:1499:C:C2     | 40:a:1500:G:C8     | 3.03                     | 0.46              |
| 40:a:1588:G:C6     | 40:a:1589:U:O4     | 2.69                     | 0.46              |
| 46:g:1:MET:SD      | 46:g:3:LYS:HE2     | 2.56                     | 0.46              |
| 48:i:52:ARG:HA     | 48:i:52:ARG:NE     | 2.30                     | 0.46              |
| 48:i:55:ILE:HD13   | 62:w:112:TYR:CE1   | 2.50                     | 0.46              |
| 54:o:31:HIS:O      | 54:o:32:ILE:O      | 2.33                     | 0.46              |
| 56:q:1:MET:HE3     | 56:q:1:MET:HA      | 1.97                     | 0.46              |
| 61:v:41:LEU:HD22   | 61:v:124:LEU:HD22  | 1.97                     | 0.46              |
| 62:w:48:VAL:CG1    | 62:w:49:GLU:OE1    | 2.64                     | 0.46              |
| 10:A:6:G:O2'       | 10:A:7:G:H8        | 1.98                     | 0.46              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 11:AA:712:SER:OG  | 11:AA:713:GLY:N     | 2.49                     | 0.46              |
| 13:AD:182:ARG:HD2 | 14:AE:581:MET:HE1   | 1.98                     | 0.46              |
| 17:D:277:C:OP1    | 35:V:43:LYS:HD2     | 2.15                     | 0.46              |
| 17:D:440:C:C2     | 17:D:441:A:C8       | 3.04                     | 0.46              |
| 17:D:520:A:O3'    | 31:R:70:GLU:OE2     | 2.32                     | 0.46              |
| 17:D:1209:C:C2    | 17:D:1210:C:C5      | 3.04                     | 0.46              |
| 17:D:1513:A:H2'   | 17:D:1514:G:C8      | 2.51                     | 0.46              |
| 19:F:63:GLU:HG2   | 19:F:67:ARG:CZ      | 2.46                     | 0.46              |
| 20:G:19:GLN:NE2   | 21:H:75:VAL:HG13    | 2.30                     | 0.46              |
| 21:H:24:VAL:HG23  | 21:H:24:VAL:O       | 2.16                     | 0.46              |
| 25:L:94:HIS:CG    | 25:L:95:ALA:H       | 2.34                     | 0.46              |
| 26:M:31:MET:HE1   | 26:M:36:LYS:CD      | 2.46                     | 0.46              |
| 26:M:44:TYR:C     | 26:M:44:TYR:CD2     | 2.94                     | 0.46              |
| 26:M:66:LEU:HD13  | 26:M:101:MET:HE3    | 1.93                     | 0.46              |
| 28:O:46:MET:HB3   | 28:O:50:GLN:NE2     | 2.31                     | 0.46              |
| 29:P:27:GLU:HA    | 29:P:30:LYS:HZ1     | 1.79                     | 0.46              |
| 32:S:12:LYS:NZ    | 32:S:16:LEU:HD21    | 2.31                     | 0.46              |
| 33:T:15:PHE:CE2   | 33:T:30:ALA:HB1     | 2.51                     | 0.46              |
| 38:Y:59:THR:C     | 38:Y:66:PHE:HB2     | 2.41                     | 0.46              |
| 40:a:392:U:C2     | 40:a:393:C:C5       | 3.03                     | 0.46              |
| 40:a:493:G:H2'    | 40:a:494:G:O4'      | 2.16                     | 0.46              |
| 40:a:1107:G:C5    | 40:a:1108:U:C5      | 3.04                     | 0.46              |
| 40:a:1421:G:C2    | 40:a:1422:G:C8      | 3.03                     | 0.46              |
| 40:a:1707:G:C4    | 40:a:1708:C:C5      | 3.04                     | 0.46              |
| 40:a:2373:G:H2'   | 40:a:2374:C:H6      | 1.81                     | 0.46              |
| 43:d:8:C:O3'      | 63:x:25:ARG:NH1     | 2.48                     | 0.46              |
| 49:j:74:GLU:HG2   | 49:j:75:ALA:N       | 2.31                     | 0.46              |
| 50:k:19:HIS:CE1   | 50:k:41:PRO:CD      | 2.99                     | 0.46              |
| 51:l:108:ILE:HD11 | 51:l:180:LEU:HD13   | 1.98                     | 0.46              |
| 54:o:26:HIS:CE1   | 54:o:48:ALA:HB2     | 2.51                     | 0.46              |
| 63:x:90:VAL:CG2   | 63:x:115:LEU:HD21   | 2.46                     | 0.46              |
| 3:2:5:GLU:HA      | 44:e:22:LEU:CD2     | 2.45                     | 0.45              |
| 5:4:50:MET:C      | 5:4:56:PHE:CZ       | 2.94                     | 0.45              |
| 5:4:53:LYS:HD2    | 5:4:56:PHE:CZ       | 2.50                     | 0.45              |
| 8:7:1:A:H2'       | 8:7:2:U:C6          | 2.50                     | 0.45              |
| 9:9:3:LEU:HD12    | 9:9:5:LEU:H         | 1.82                     | 0.45              |
| 9:9:34:THR:HA     | 9:9:37:LYS:NZ       | 2.32                     | 0.45              |
| 11:AA:689:ALA:HB2 | 11:AA:1233:LEU:HD23 | 1.97                     | 0.45              |
| 11:AA:735:LYS:HA  | 11:AA:748:ILE:HG22  | 1.98                     | 0.45              |
| 11:AA:1314:GLN:HA | 15:AF:28:ARG:HH22   | 1.80                     | 0.45              |
| 14:AE:420:PRO:HA  | 14:AE:437:PHE:O     | 2.16                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 16:C:12:ARG:NH2    | 16:C:28:THR:CG2   | 2.79                     | 0.45              |
| 16:C:12:ARG:HB2    | 21:H:264:GLU:CB   | 2.46                     | 0.45              |
| 16:C:14:THR:HG21   | 16:C:48:ARG:CD    | 2.46                     | 0.45              |
| 17:D:723:U:O2      | 19:F:49:LYS:HE3   | 2.16                     | 0.45              |
| 17:D:765:G:C6      | 17:D:812:G:C4     | 3.04                     | 0.45              |
| 17:D:878:A:P       | 27:N:80:ARG:HH11  | 2.39                     | 0.45              |
| 17:D:1173:U:H2'    | 17:D:1174:G:O4'   | 2.16                     | 0.45              |
| 17:D:1202:U:C5     | 17:D:1203:C:C5    | 3.05                     | 0.45              |
| 21:H:115:LYS:HA    | 21:H:119:GLY:C    | 2.40                     | 0.45              |
| 24:K:13:GLU:O      | 24:K:13:GLU:HG2   | 2.16                     | 0.45              |
| 24:K:86:LYS:HE3    | 24:K:95:PHE:CD1   | 2.50                     | 0.45              |
| 25:L:98:GLU:HA     | 25:L:98:GLU:OE1   | 2.16                     | 0.45              |
| 26:M:16:PRO:CB     | 28:O:46:MET:HG3   | 2.42                     | 0.45              |
| 26:M:78:ARG:CG     | 26:M:80:VAL:HG13  | 2.46                     | 0.45              |
| 27:N:89:LYS:HG3    | 27:N:90:ASP:N     | 2.31                     | 0.45              |
| 29:P:59:LYS:HE2    | 29:P:62:ARG:NH2   | 2.31                     | 0.45              |
| 29:P:63:ASP:OD2    | 29:P:63:ASP:C     | 2.59                     | 0.45              |
| 31:R:68:GLY:O      | 31:R:99:ARG:NH1   | 2.48                     | 0.45              |
| 32:S:77:PHE:CE1    | 32:S:93:ILE:HD13  | 2.51                     | 0.45              |
| 38:Y:102:ARG:HE    | 38:Y:139:VAL:HG21 | 1.79                     | 0.45              |
| 38:Y:126:ARG:HH12  | 40:a:1082:U:C5'   | 2.29                     | 0.45              |
| 40:a:67:U:N3       | 40:a:68:G:C5      | 2.84                     | 0.45              |
| 40:a:306:U:H2'     | 40:a:307:G:O4'    | 2.16                     | 0.45              |
| 40:a:396:G:C5      | 40:a:397:U:C5     | 3.03                     | 0.45              |
| 40:a:644:A:C2      | 40:a:2369:A:H1'   | 2.51                     | 0.45              |
| 40:a:1065:U:HO2'   | 40:a:1066:U:C5'   | 2.26                     | 0.45              |
| 40:a:1406:U:O2     | 40:a:1407:G:C8    | 2.69                     | 0.45              |
| 40:a:2289:G:C2     | 40:a:2290:G:C8    | 3.04                     | 0.45              |
| 40:a:2756:U:N3     | 40:a:2758:A:N6    | 2.64                     | 0.45              |
| 41:b:26:PHE:O      | 41:b:29:GLU:HG2   | 2.15                     | 0.45              |
| 54:o:49:MET:H      | 54:o:49:MET:HE2   | 1.82                     | 0.45              |
| 55:p:11:VAL:HG13   | 55:p:11:VAL:O     | 2.17                     | 0.45              |
| 56:q:30:GLU:HB3    | 56:q:33:HIS:ND1   | 2.32                     | 0.45              |
| 62:w:115:LEU:HD23  | 62:w:117:ASP:N    | 2.30                     | 0.45              |
| 64:y:103:ARG:HD3   | 64:y:107:ALA:C    | 2.41                     | 0.45              |
| 64:y:106:LYS:CD    | 64:y:109:ARG:NH2  | 2.79                     | 0.45              |
| 9:9:94:ARG:CB      | 9:9:97:LYS:CE     | 2.94                     | 0.45              |
| 10:A:46:G:H1'      | 10:A:47:U:C5      | 2.51                     | 0.45              |
| 11:AA:400:VAL:HG22 | 11:AA:584:TYR:HB3 | 1.96                     | 0.45              |
| 17:D:13:U:O2       | 17:D:915:A:N7     | 2.49                     | 0.45              |
| 17:D:413:G:N2      | 17:D:428:G:H1'    | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:D:653:U:N1     | 27:N:56:LYS:HE3   | 2.30                     | 0.45              |
| 17:D:829:G:H4'    | 20:G:23:TRP:CH2   | 2.51                     | 0.45              |
| 17:D:984:C:C2     | 17:D:985:C:C5     | 3.05                     | 0.45              |
| 17:D:1132:C:O2    | 17:D:1132:C:H2'   | 2.16                     | 0.45              |
| 21:H:288:THR:O    | 21:H:288:THR:HG22 | 2.16                     | 0.45              |
| 25:L:9:MET:C      | 25:L:9:MET:SD     | 3.00                     | 0.45              |
| 25:L:35:LYS:HD2   | 25:L:36:ILE:H     | 1.82                     | 0.45              |
| 27:N:8:ALA:N      | 27:N:77:ARG:HH11  | 2.14                     | 0.45              |
| 27:N:25:VAL:HG23  | 27:N:63:LEU:CD1   | 2.47                     | 0.45              |
| 28:O:88:MET:CE    | 28:O:95:ARG:HG3   | 2.46                     | 0.45              |
| 31:R:18:LYS:HD3   | 31:R:19:SER:O     | 2.16                     | 0.45              |
| 32:S:82:ILE:HG23  | 32:S:83:LYS:N     | 2.31                     | 0.45              |
| 37:X:104:THR:O    | 37:X:104:THR:HG22 | 2.16                     | 0.45              |
| 38:Y:102:ARG:HD3  | 38:Y:141:ASP:OD1  | 2.15                     | 0.45              |
| 40:a:247:G:O6     | 54:o:12:LYS:NZ    | 2.39                     | 0.45              |
| 40:a:2049:G:N2    | 49:j:161:MET:CE   | 2.80                     | 0.45              |
| 40:a:2065:C:C2    | 40:a:2066:C:C5    | 3.04                     | 0.45              |
| 40:a:2309:A:H2'   | 40:a:2310:C:O4'   | 2.16                     | 0.45              |
| 42:c:30:LEU:CD1   | 42:c:31:PRO:HD2   | 2.43                     | 0.45              |
| 48:i:30:VAL:HG22  | 48:i:37:LYS:HD2   | 1.98                     | 0.45              |
| 51:l:23:PHE:CD1   | 51:l:111:GLU:CD   | 2.95                     | 0.45              |
| 51:l:149:ILE:CD1  | 51:l:188:MET:HG2  | 2.46                     | 0.45              |
| 56:q:1:MET:HE3    | 56:q:2:LYS:N      | 2.31                     | 0.45              |
| 58:s:73:VAL:CG1   | 58:s:86:GLN:HG2   | 2.46                     | 0.45              |
| 59:t:108:ARG:CG   | 59:t:116:ILE:HD13 | 2.46                     | 0.45              |
| 63:x:15:ARG:C     | 63:x:19:GLN:HE22  | 2.23                     | 0.45              |
| 65:z:89:GLU:N     | 65:z:89:GLU:OE1   | 2.50                     | 0.45              |
| 2:1:11:ARG:NH1    | 2:1:11:ARG:HB3    | 2.30                     | 0.45              |
| 2:1:20:VAL:CG1    | 2:1:47:VAL:HG11   | 2.46                     | 0.45              |
| 3:2:64:LYS:CE     | 40:a:1312:U:O4    | 2.64                     | 0.45              |
| 7:6:25:DT:H2'     | 11:AA:496:LYS:CG  | 2.44                     | 0.45              |
| 9:9:23:LEU:HA     | 9:9:118:ILE:HD11  | 1.99                     | 0.45              |
| 11:AA:557:ARG:NH2 | 11:AA:607:SER:O   | 2.49                     | 0.45              |
| 11:AA:812:PHE:HZ  | 14:AE:503:SER:HB2 | 1.81                     | 0.45              |
| 12:AB:141:LEU:HB2 | 12:AB:153:SER:OG  | 2.16                     | 0.45              |
| 14:AE:41:PRO:HB2  | 14:AE:270:ARG:HG3 | 1.99                     | 0.45              |
| 14:AE:53:ARG:HA   | 14:AE:54:ASP:HA   | 1.59                     | 0.45              |
| 14:AE:68:TYR:CA   | 14:AE:92:VAL:HG23 | 2.45                     | 0.45              |
| 10:B:32:C:C2'     | 10:B:33:U:H5'     | 2.46                     | 0.45              |
| 17:D:269:C:H2'    | 17:D:270:A:C8     | 2.51                     | 0.45              |
| 17:D:377:G:H2'    | 17:D:378:G:H8     | 1.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:D:1108:G:C5    | 17:D:1109:C:C5    | 3.04                     | 0.45              |
| 17:D:1315:U:O2    | 17:D:1360:A:H2    | 2.00                     | 0.45              |
| 18:E:54:MET:O     | 18:E:58:VAL:HG23  | 2.16                     | 0.45              |
| 20:G:117:LEU:HD23 | 20:G:141:LEU:HA   | 1.98                     | 0.45              |
| 21:H:32:ASP:OD1   | 21:H:35:VAL:HG23  | 2.17                     | 0.45              |
| 24:K:145:GLU:CD   | 24:K:146:ASN:N    | 2.74                     | 0.45              |
| 25:L:38:ARG:NE    | 25:L:97:THR:O     | 2.49                     | 0.45              |
| 26:M:132:GLY:O    | 26:M:136:LYS:HD3  | 2.17                     | 0.45              |
| 26:M:134:ALA:HA   | 26:M:137:LYS:CD   | 2.46                     | 0.45              |
| 29:P:26:VAL:C     | 29:P:30:LYS:HZ3   | 2.25                     | 0.45              |
| 31:R:110:ARG:N    | 31:R:111:LYS:HZ3  | 2.15                     | 0.45              |
| 34:U:73:ALA:HA    | 34:U:76:LYS:HE3   | 1.98                     | 0.45              |
| 36:W:44:MET:HE1   | 36:W:62:VAL:CG2   | 2.46                     | 0.45              |
| 37:X:13:LYS:HZ2   | 37:X:17:ILE:HG21  | 1.81                     | 0.45              |
| 37:X:56:LEU:HA    | 37:X:59:GLU:OE1   | 2.16                     | 0.45              |
| 38:Y:45:THR:HG22  | 38:Y:45:THR:O     | 2.16                     | 0.45              |
| 40:a:219:A:H2'    | 40:a:220:G:C8     | 2.52                     | 0.45              |
| 40:a:235:U:N3     | 40:a:236:C:C5     | 2.84                     | 0.45              |
| 40:a:669:G:H2'    | 40:a:670:A:N7     | 2.31                     | 0.45              |
| 40:a:893:C:H2'    | 40:a:894:U:C5     | 2.51                     | 0.45              |
| 40:a:952:G:C6     | 40:a:966:G:C6     | 3.04                     | 0.45              |
| 40:a:1370:C:H2'   | 40:a:1371:G:O4'   | 2.16                     | 0.45              |
| 40:a:1408:G:N3    | 40:a:1408:G:H2'   | 2.31                     | 0.45              |
| 40:a:1796:U:H2'   | 40:a:1797:G:H8    | 1.81                     | 0.45              |
| 40:a:2364:C:H2'   | 40:a:2365:G:O4'   | 2.15                     | 0.45              |
| 40:a:2814:A:C5    | 40:a:2815:C:C5    | 3.05                     | 0.45              |
| 46:g:16:CYS:SG    | 46:g:37:CYS:N     | 2.89                     | 0.45              |
| 47:h:33:LEU:O     | 47:h:64:ILE:HG12  | 2.16                     | 0.45              |
| 49:j:5:VAL:HG22   | 49:j:202:ILE:CD1  | 2.46                     | 0.45              |
| 49:j:5:VAL:HB     | 49:j:32:ASN:ND2   | 2.31                     | 0.45              |
| 51:l:21:ARG:HA    | 51:l:21:ARG:NE    | 2.31                     | 0.45              |
| 55:p:91:GLY:HA3   | 55:p:94:TYR:CD2   | 2.52                     | 0.45              |
| 57:r:31:VAL:HB    | 57:r:32:PRO:HD3   | 1.97                     | 0.45              |
| 59:t:76:VAL:HG12  | 64:y:73:VAL:HB    | 1.97                     | 0.45              |
| 64:y:106:LYS:CD   | 64:y:109:ARG:HH22 | 2.29                     | 0.45              |
| 3:2:65:GLY:H      | 3:2:76:ARG:HH12   | 1.64                     | 0.45              |
| 4:3:46:GLN:NE2    | 4:3:54:GLN:HG2    | 2.31                     | 0.45              |
| 4:3:47:LYS:HZ3    | 40:a:482:A:P      | 2.40                     | 0.45              |
| 4:3:66:GLN:OE1    | 40:a:329:G:OP2    | 2.34                     | 0.45              |
| 9:9:11:ILE:HG12   | 9:9:65:GLU:HG2    | 1.98                     | 0.45              |
| 9:9:61:ARG:CD     | 40:a:1046:A:O5'   | 2.64                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:D:511:C:C2     | 17:D:512:U:C5     | 3.05                     | 0.45              |
| 17:D:696:A:H2'    | 17:D:697:U:H6     | 1.81                     | 0.45              |
| 17:D:736:C:H5'    | 25:L:90:MET:HE2   | 1.97                     | 0.45              |
| 19:F:38:TYR:O     | 30:Q:126:LYS:HE3  | 2.17                     | 0.45              |
| 28:O:113:ARG:HD2  | 32:S:101:TRP:CD1  | 2.52                     | 0.45              |
| 31:R:31:ARG:O     | 31:R:57:LEU:HD12  | 2.17                     | 0.45              |
| 33:T:8:THR:O      | 33:T:11:ILE:HG22  | 2.16                     | 0.45              |
| 33:T:15:PHE:HE2   | 33:T:30:ALA:HB1   | 1.82                     | 0.45              |
| 37:X:55:THR:C     | 37:X:59:GLU:OE1   | 2.60                     | 0.45              |
| 38:Y:19:PRO:HG2   | 38:Y:23:VAL:CG2   | 2.42                     | 0.45              |
| 38:Y:79:LEU:O     | 38:Y:83:ALA:HB3   | 2.16                     | 0.45              |
| 38:Y:102:ARG:HH21 | 38:Y:105:LEU:HD12 | 1.81                     | 0.45              |
| 38:Y:126:ARG:HH12 | 40:a:1083:U:P     | 2.40                     | 0.45              |
| 40:a:590:A:H2'    | 40:a:591:U:H6     | 1.80                     | 0.45              |
| 40:a:607:U:C6     | 40:a:620:G:C5     | 3.04                     | 0.45              |
| 40:a:783:A:O2'    | 40:a:785:G:OP1    | 2.35                     | 0.45              |
| 40:a:923:G:H4'    | 41:b:29:GLU:OE1   | 2.16                     | 0.45              |
| 40:a:1131:G:OP1   | 58:s:81:ILE:O     | 2.34                     | 0.45              |
| 40:a:2149:U:H2'   | 40:a:2150:C:C6    | 2.52                     | 0.45              |
| 40:a:2848:G:C2    | 40:a:2867:G:C4    | 3.05                     | 0.45              |
| 43:d:57:A:C5      | 53:n:26:MET:CE    | 2.99                     | 0.45              |
| 45:f:12:SER:CA    | 45:f:32:ILE:HD11  | 2.46                     | 0.45              |
| 49:j:48:ILE:CD1   | 49:j:84:LEU:HD11  | 2.46                     | 0.45              |
| 49:j:55:LYS:NZ    | 49:j:56:LYS:O     | 2.49                     | 0.45              |
| 50:k:7:GLU:OE2    | 50:k:27:LYS:HG3   | 2.16                     | 0.45              |
| 51:l:95:LYS:HE2   | 51:l:97:ASN:OD1   | 2.17                     | 0.45              |
| 52:m:12:ARG:CG    | 52:m:44:VAL:HG21  | 2.47                     | 0.45              |
| 55:p:85:LYS:HA    | 55:p:85:LYS:HD2   | 1.77                     | 0.45              |
| 56:q:1:MET:HE1    | 56:q:35:GLN:HA    | 1.95                     | 0.45              |
| 63:x:35:ILE:HD11  | 63:x:102:ARG:HH21 | 1.81                     | 0.45              |
| 7:6:25:DT:OP1     | 11:AA:496:LYS:O   | 2.34                     | 0.45              |
| 10:A:71:C:C3'     | 10:A:72:A:C8      | 2.99                     | 0.45              |
| 10:B:6:G:O2'      | 10:B:7:G:H8       | 1.98                     | 0.45              |
| 10:B:53:G:N3      | 10:B:54:U:C5      | 2.85                     | 0.45              |
| 17:D:110:C:H1'    | 34:U:25:ARG:NH1   | 2.31                     | 0.45              |
| 17:D:878:A:P      | 27:N:80:ARG:NH1   | 2.89                     | 0.45              |
| 17:D:1287:A:H2'   | 17:D:1288:A:C8    | 2.52                     | 0.45              |
| 18:E:54:MET:C     | 18:E:54:MET:SD    | 3.00                     | 0.45              |
| 19:F:12:PHE:CD1   | 30:Q:101:ASN:CG   | 2.95                     | 0.45              |
| 20:G:27:MET:HG3   | 20:G:27:MET:O     | 2.16                     | 0.45              |
| 20:G:128:LYS:C    | 20:G:129:LEU:HD12 | 2.42                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 21:H:32:ASP:OD1     | 21:H:35:VAL:HG22   | 2.17                     | 0.45              |
| 22:I:39:VAL:HG23    | 22:I:40:ARG:N      | 2.32                     | 0.45              |
| 22:I:84:VAL:HG23    | 22:I:85:GLU:N      | 2.31                     | 0.45              |
| 22:I:142:MET:HE3    | 22:I:170:GLU:HB3   | 1.98                     | 0.45              |
| 25:L:18:VAL:N       | 25:L:19:PRO:CD     | 2.80                     | 0.45              |
| 26:M:134:ALA:O      | 26:M:137:LYS:CG    | 2.65                     | 0.45              |
| 28:O:51:PRO:CA      | 28:O:103:PHE:HE2   | 2.30                     | 0.45              |
| 34:U:45:GLU:HG3     | 34:U:46:LYS:CD     | 2.45                     | 0.45              |
| 40:a:78:U:P         | 44:e:4:LYS:NZ      | 2.89                     | 0.45              |
| 40:a:532:A:OP1      | 65:z:45:TYR:OH     | 2.32                     | 0.45              |
| 40:a:685:A:C8       | 40:a:773:U:C4      | 3.04                     | 0.45              |
| 40:a:837:C:N3       | 40:a:941:A:N6      | 2.65                     | 0.45              |
| 40:a:1790:C:C2'     | 40:a:1791:A:C8     | 3.00                     | 0.45              |
| 40:a:2061:G:N2      | 40:a:2063:C:C6     | 2.84                     | 0.45              |
| 40:a:2095:A:O5'     | 57:r:11:ASN:OD1    | 2.35                     | 0.45              |
| 40:a:2262:U:N3      | 40:a:2263:C:C5     | 2.85                     | 0.45              |
| 40:a:2529:G:N7      | 56:q:32:LYS:NZ     | 2.63                     | 0.45              |
| 40:a:2743:U:H2'     | 40:a:2744:G:O4'    | 2.17                     | 0.45              |
| 49:j:71:ALA:HB3     | 49:j:73:VAL:HG22   | 1.98                     | 0.45              |
| 53:n:127:ASN:OD1    | 53:n:157:THR:HA    | 2.16                     | 0.45              |
| 53:n:142:ASP:CB     | 53:n:145:LYS:HE2   | 2.40                     | 0.45              |
| 54:o:55:LEU:CD2     | 54:o:59:ILE:HD11   | 2.46                     | 0.45              |
| 57:r:135:HIS:CE1    | 57:r:137:GLU:OE1   | 2.62                     | 0.45              |
| 2:1:20:VAL:HG11     | 2:1:47:VAL:HG11    | 1.99                     | 0.45              |
| 3:2:64:LYS:HD2      | 40:a:1312:U:C4     | 2.51                     | 0.45              |
| 9:9:61:ARG:HE       | 40:a:1046:A:P      | 2.39                     | 0.45              |
| 9:9:122:GLN:OE1     | 9:9:122:GLN:N      | 2.49                     | 0.45              |
| 10:A:68:C:H3'       | 10:A:69:C:H5''     | 1.97                     | 0.45              |
| 11:AA:1002:LEU:HD21 | 11:AA:1007:LYS:HB2 | 1.98                     | 0.45              |
| 12:AB:6:LEU:N       | 12:AB:88:VAL:HG21  | 2.31                     | 0.45              |
| 14:AE:781:LYS:HD2   | 14:AE:933:ARG:HH12 | 1.81                     | 0.45              |
| 10:B:46:G:H1'       | 10:B:47:U:C5       | 2.51                     | 0.45              |
| 17:D:983:A:H2       | 17:D:984:C:C6      | 2.34                     | 0.45              |
| 19:F:58:LYS:HD2     | 19:F:58:LYS:C      | 2.42                     | 0.45              |
| 20:G:109:GLN:C      | 20:G:113:ARG:NE    | 2.75                     | 0.45              |
| 22:I:72:ARG:NE      | 22:I:75:ILE:HB     | 2.32                     | 0.45              |
| 22:I:114:LYS:HB2    | 22:I:185:ASN:ND2   | 2.32                     | 0.45              |
| 23:J:76:TYR:HE2     | 23:J:204:TYR:CB    | 2.25                     | 0.45              |
| 24:K:13:GLU:OE1     | 24:K:13:GLU:N      | 2.49                     | 0.45              |
| 25:L:100:SER:HB2    | 25:L:101:PRO:HD2   | 1.98                     | 0.45              |
| 26:M:87:VAL:HG12    | 26:M:151:PHE:HD2   | 1.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:P:47:GLU:HB2   | 29:P:67:ILE:HG22  | 1.99                     | 0.45              |
| 30:Q:88:GLY:H     | 30:Q:114:THR:HG22 | 1.81                     | 0.45              |
| 31:R:30:LYS:O     | 31:R:81:LEU:HD12  | 2.16                     | 0.45              |
| 33:T:15:PHE:CE2   | 33:T:30:ALA:CB    | 3.00                     | 0.45              |
| 36:W:13:LEU:O     | 36:W:17:LYS:HG2   | 2.17                     | 0.45              |
| 37:X:14:HIS:HB2   | 37:X:17:ILE:HD13  | 1.99                     | 0.45              |
| 38:Y:93:ASN:O     | 38:Y:94:LYS:HD2   | 2.16                     | 0.45              |
| 40:a:132:G:H2'    | 40:a:133:U:H6     | 1.81                     | 0.45              |
| 40:a:1019:U:O4    | 40:a:1142:A:C2    | 2.69                     | 0.45              |
| 40:a:1444:G:C4    | 40:a:1445:G:C8    | 3.05                     | 0.45              |
| 40:a:1797:G:O2'   | 47:h:257:THR:HG22 | 2.16                     | 0.45              |
| 40:a:2478:A:C8    | 40:a:2529:G:C5    | 3.04                     | 0.45              |
| 40:a:2727:A:O3'   | 59:t:70:ARG:NH2   | 2.50                     | 0.45              |
| 43:d:45:A:C5'     | 53:n:92:ARG:NH1   | 2.79                     | 0.45              |
| 45:f:12:SER:C     | 45:f:54:MET:HE1   | 2.40                     | 0.45              |
| 49:j:146:ILE:HA   | 49:j:159:LYS:HZ1  | 1.82                     | 0.45              |
| 51:l:60:TRP:CD1   | 51:l:69:ARG:HH12  | 2.33                     | 0.45              |
| 55:p:11:VAL:HG12  | 55:p:48:ASN:O     | 2.17                     | 0.45              |
| 55:p:149:ARG:CZ   | 55:p:162:VAL:C    | 2.89                     | 0.45              |
| 60:u:101:ILE:C    | 60:u:105:ILE:HD12 | 2.42                     | 0.45              |
| 60:u:103:ILE:HG23 | 60:u:104:GLN:HG2  | 1.99                     | 0.45              |
| 62:w:20:MET:HE3   | 62:w:20:MET:HB2   | 1.83                     | 0.45              |
| 64:y:15:GLN:NE2   | 64:y:16:ASP:CG    | 2.75                     | 0.45              |
| 64:y:31:TRP:CZ3   | 64:y:40:LEU:CD1   | 3.00                     | 0.45              |
| 65:z:76:TYR:O     | 65:z:80:ILE:HG12  | 2.16                     | 0.45              |
| 2:1:24:ILE:HG21   | 2:1:36:LEU:CD1    | 2.42                     | 0.45              |
| 2:1:78:GLU:OE2    | 40:a:1262:A:OP1   | 2.35                     | 0.45              |
| 5:4:57:TYR:HD2    | 61:v:136:MET:HE2  | 1.82                     | 0.45              |
| 8:7:2:U:OP2       | 17:D:926:G:N2     | 2.50                     | 0.45              |
| 11:AA:746:ALA:O   | 11:AA:974:ARG:NH2 | 2.45                     | 0.45              |
| 12:AB:160:ARG:HG3 | 12:AB:161:LYS:N   | 2.32                     | 0.45              |
| 13:AD:35:PHE:HA   | 13:AD:38:THR:HG22 | 1.97                     | 0.45              |
| 14:AE:640:GLY:N   | 14:AE:643:ASP:OD2 | 2.42                     | 0.45              |
| 17:D:13:U:O4      | 17:D:20:U:O4      | 2.34                     | 0.45              |
| 17:D:653:U:O4'    | 27:N:56:LYS:HE3   | 2.16                     | 0.45              |
| 17:D:915:A:C5     | 17:D:916:U:C5     | 3.04                     | 0.45              |
| 17:D:918:A:H2'    | 17:D:919:A:C8     | 2.51                     | 0.45              |
| 17:D:980:C:C5     | 17:D:981:U:C2     | 3.04                     | 0.45              |
| 20:G:19:GLN:HE21  | 21:H:75:VAL:C     | 2.24                     | 0.45              |
| 20:G:77:SER:O     | 20:G:80:VAL:HG12  | 2.17                     | 0.45              |
| 21:H:37:LEU:HG    | 21:H:46:SER:O     | 2.17                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 21:H:54:LYS:HD3     | 21:H:58:GLY:C      | 2.42                     | 0.45              |
| 24:K:86:LYS:HZ2     | 24:K:95:PHE:HE1    | 1.65                     | 0.45              |
| 26:M:138:ARG:HG2    | 26:M:142:HIS:HE1   | 1.81                     | 0.45              |
| 26:M:138:ARG:O      | 26:M:142:HIS:ND1   | 2.46                     | 0.45              |
| 28:O:5:GLN:HE21     | 28:O:20:PHE:HB3    | 1.81                     | 0.45              |
| 28:O:80:ARG:NH2     | 28:O:103:PHE:CE1   | 2.85                     | 0.45              |
| 37:X:55:THR:HG22    | 37:X:59:GLU:OE2    | 2.17                     | 0.45              |
| 40:a:535:G:H2'      | 40:a:536:G:O4'     | 2.17                     | 0.45              |
| 40:a:582:A:H5''     | 65:z:11:ARG:HH12   | 1.82                     | 0.45              |
| 40:a:1656:C:H2'     | 40:a:1657:U:H6     | 1.81                     | 0.45              |
| 40:a:1665:A:C5'     | 59:t:66:LYS:NZ     | 2.79                     | 0.45              |
| 40:a:1889:A:H2'     | 40:a:1890:A:C8     | 2.51                     | 0.45              |
| 40:a:2064:C:H2'     | 40:a:2065:C:H6     | 1.80                     | 0.45              |
| 40:a:2649:C:H2'     | 40:a:2650:U:C6     | 2.51                     | 0.45              |
| 40:a:2723:C:H2'     | 40:a:2724:U:O4'    | 2.16                     | 0.45              |
| 40:a:2766:A:C6      | 40:a:2767:C:C5     | 3.05                     | 0.45              |
| 51:l:73:ILE:HG13    | 51:l:73:ILE:O      | 2.17                     | 0.45              |
| 59:t:1:MET:CE       | 59:t:32:TYR:CG     | 2.99                     | 0.45              |
| 59:t:17:ARG:NH2     | 59:t:47:ILE:CG2    | 2.80                     | 0.45              |
| 62:w:56:LYS:NZ      | 62:w:90:ARG:O      | 2.47                     | 0.45              |
| 4:3:5:ILE:HG13      | 4:3:72:ILE:HD11    | 1.99                     | 0.45              |
| 5:4:16:ALA:O        | 5:4:20:LEU:HG      | 2.17                     | 0.45              |
| 8:7:25:G:O2'        | 14:AE:394:ILE:CG2  | 2.64                     | 0.45              |
| 10:A:3:C:H2'        | 10:A:4:G:H8        | 1.82                     | 0.45              |
| 11:AA:1246:ARG:HH11 | 11:AA:1266:GLY:HA2 | 1.82                     | 0.45              |
| 12:AB:52:PRO:O      | 12:AB:54:TYR:N     | 2.50                     | 0.45              |
| 14:AE:482:ALA:HA    | 15:AF:6:VAL:HG21   | 1.98                     | 0.45              |
| 17:D:636:U:H2'      | 17:D:637:C:C6      | 2.52                     | 0.45              |
| 17:D:1006:G:H2'     | 17:D:1007:U:H6     | 1.81                     | 0.45              |
| 17:D:1086:U:O2      | 17:D:1086:U:H2'    | 2.16                     | 0.45              |
| 17:D:1323:G:H2'     | 17:D:1324:A:H8     | 1.78                     | 0.45              |
| 20:G:66:LYS:HB3     | 20:G:154:MET:HE3   | 1.99                     | 0.45              |
| 21:H:53:PHE:CE1     | 21:H:68:VAL:HG21   | 2.52                     | 0.45              |
| 27:N:26:THR:OG1     | 27:N:58:GLU:CG     | 2.65                     | 0.45              |
| 37:X:11:ASP:HA      | 37:X:45:ILE:HB     | 1.99                     | 0.45              |
| 37:X:90:ARG:HD3     | 37:X:96:PRO:O      | 2.17                     | 0.45              |
| 38:Y:5:GLN:NE2      | 38:Y:60:VAL:C      | 2.74                     | 0.45              |
| 38:Y:126:ARG:NH2    | 40:a:1082:U:O3'    | 2.47                     | 0.45              |
| 40:a:111:A:O2'      | 44:e:58:ASN:ND2    | 2.46                     | 0.45              |
| 40:a:372:G:O2'      | 42:c:54:LYS:CE     | 2.64                     | 0.45              |
| 40:a:598:U:H2'      | 40:a:599:A:C8      | 2.52                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:a:1042:G:C5     | 40:a:1043:C:C5     | 3.05                     | 0.45              |
| 40:a:1856:U:H2'    | 40:a:1857:G:O4'    | 2.17                     | 0.45              |
| 40:a:2356:U:H4'    | 41:b:20:ARG:HD2    | 1.99                     | 0.45              |
| 40:a:2683:C:OP1    | 64:y:51:ARG:NH2    | 2.46                     | 0.45              |
| 44:e:24:GLU:O      | 44:e:28:LEU:HD13   | 2.17                     | 0.45              |
| 45:f:51:VAL:O      | 45:f:55:VAL:HG12   | 2.17                     | 0.45              |
| 51:l:194:LYS:HG3   | 51:l:198:GLU:OE2   | 2.16                     | 0.45              |
| 53:n:22:TYR:CE2    | 53:n:28:VAL:HA     | 2.52                     | 0.45              |
| 53:n:122:PHE:HZ    | 53:n:170:LEU:HD12  | 1.81                     | 0.45              |
| 59:t:24:VAL:HG23   | 59:t:33:ALA:HB2    | 1.97                     | 0.45              |
| 60:u:91:ASP:HB2    | 60:u:93:ASN:OD1    | 2.17                     | 0.45              |
| 62:w:12:ARG:HE     | 62:w:20:MET:HE1    | 1.82                     | 0.45              |
| 2:1:86:MET:SD      | 2:1:88:ARG:HD2     | 2.56                     | 0.45              |
| 5:4:29:ILE:HD13    | 43:d:74:U:O2       | 2.17                     | 0.45              |
| 5:4:31:TYR:O       | 5:4:92:VAL:HA      | 2.17                     | 0.45              |
| 5:4:50:MET:CB      | 5:4:56:PHE:CE1     | 2.98                     | 0.45              |
| 9:9:4:ASN:HB3      | 9:9:8:LYS:HZ2      | 1.80                     | 0.45              |
| 9:9:14:GLU:OE1     | 9:9:63:ALA:HA      | 2.17                     | 0.45              |
| 9:9:68:PRO:O       | 9:9:72:LEU:HD21    | 2.16                     | 0.45              |
| 9:9:87:GLU:OE2     | 9:9:95:LEU:CG      | 2.64                     | 0.45              |
| 11:AA:28:LEU:HD21  | 11:AA:524:ILE:HG13 | 1.97                     | 0.45              |
| 11:AA:176:ILE:HD11 | 11:AA:428:VAL:HG21 | 1.98                     | 0.45              |
| 12:AB:6:LEU:CD2    | 14:AE:291:ILE:HD11 | 2.46                     | 0.45              |
| 12:AB:76:SER:O     | 12:AB:77:HIS:HB3   | 2.16                     | 0.45              |
| 12:AB:146:ILE:HD11 | 29:P:88:MET:CB     | 2.47                     | 0.45              |
| 13:AD:68:TYR:HE1   | 13:AD:79:LEU:HD13  | 1.82                     | 0.45              |
| 14:AE:774:ILE:HA   | 14:AE:777:HIS:HD2  | 1.82                     | 0.45              |
| 14:AE:848:VAL:HB   | 14:AE:858:VAL:HG22 | 1.98                     | 0.45              |
| 10:B:3:C:H2'       | 10:B:4:G:H8        | 1.82                     | 0.45              |
| 16:C:65:LEU:HD23   | 16:C:67:LEU:CD1    | 2.47                     | 0.45              |
| 17:D:1060:U:H5''   | 29:P:53:ILE:HD12   | 1.99                     | 0.45              |
| 17:D:1240:U:OP1    | 26:M:116:MET:HB2   | 2.17                     | 0.45              |
| 21:H:303:LEU:O     | 21:H:304:VAL:C     | 2.59                     | 0.45              |
| 29:P:90:LEU:HD12   | 29:P:90:LEU:N      | 2.31                     | 0.45              |
| 32:S:13:ARG:HB3    | 32:S:60:GLN:HE21   | 1.81                     | 0.45              |
| 32:S:86:GLU:OE2    | 32:S:90:ARG:HD3    | 2.16                     | 0.45              |
| 37:X:2:ALA:HB1     | 37:X:9:ILE:CG2     | 2.47                     | 0.45              |
| 40:a:152:A:H2'     | 40:a:153:U:C6      | 2.51                     | 0.45              |
| 40:a:1613:G:O2'    | 52:m:3:ARG:CZ      | 2.64                     | 0.45              |
| 40:a:1753:G:N2     | 40:a:1755:A:H3'    | 2.32                     | 0.45              |
| 40:a:2755:C:H3'    | 56:q:19:ARG:NH2    | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:f:27:LEU:O     | 45:f:38:ARG:NE    | 2.44                     | 0.45              |
| 49:j:3:GLY:O      | 49:j:82:PHE:CE2   | 2.69                     | 0.45              |
| 53:n:4:LEU:HD21   | 53:n:101:GLU:HG3  | 1.98                     | 0.45              |
| 53:n:16:LEU:HD11  | 53:n:169:LEU:HD13 | 1.99                     | 0.45              |
| 55:p:18:LYS:HG3   | 55:p:27:LYS:NZ    | 2.32                     | 0.45              |
| 9:9:6:GLN:CA      | 9:9:9:GLN:NE2     | 2.78                     | 0.45              |
| 10:A:48:C:O2'     | 10:A:49:G:OP2     | 2.27                     | 0.45              |
| 12:AB:130:PHE:HA  | 12:AB:152:HIS:HE2 | 1.77                     | 0.45              |
| 14:AE:388:ARG:NH2 | 14:AE:414:GLU:OE1 | 2.49                     | 0.45              |
| 10:B:71:C:H2'     | 10:B:72:A:N9      | 2.32                     | 0.45              |
| 17:D:151:A:C5     | 17:D:152:A:C8     | 3.04                     | 0.45              |
| 17:D:1389:C:H2'   | 17:D:1390:U:O4'   | 2.17                     | 0.45              |
| 20:G:101:LEU:HD22 | 20:G:157:LEU:HD12 | 1.99                     | 0.45              |
| 21:H:49:PRO:CD    | 21:H:84:LEU:HD21  | 2.47                     | 0.45              |
| 22:I:14:ILE:HG13  | 22:I:178:LEU:HD21 | 1.99                     | 0.45              |
| 22:I:58:GLU:OE1   | 22:I:65:ARG:CZ    | 2.65                     | 0.45              |
| 22:I:135:LYS:O    | 22:I:138:VAL:HG12 | 2.17                     | 0.45              |
| 25:L:72:ASP:O     | 25:L:76:THR:HG23  | 2.17                     | 0.45              |
| 28:O:86:ALA:O     | 28:O:89:GLU:CG    | 2.65                     | 0.45              |
| 29:P:5:ARG:HE     | 29:P:7:ARG:CZ     | 2.29                     | 0.45              |
| 29:P:28:THR:HG22  | 29:P:90:LEU:HD23  | 1.98                     | 0.45              |
| 29:P:64:GLN:HG2   | 32:S:101:TRP:CH2  | 2.52                     | 0.45              |
| 31:R:122:PRO:C    | 31:R:123:LYS:HE2  | 2.41                     | 0.45              |
| 33:T:11:ILE:HD13  | 33:T:31:LEU:HA    | 1.99                     | 0.45              |
| 34:U:6:LEU:HD23   | 34:U:17:TYR:CB    | 2.47                     | 0.45              |
| 36:W:44:MET:HE1   | 36:W:66:MET:HE1   | 1.98                     | 0.45              |
| 37:X:16:VAL:HG23  | 37:X:17:ILE:CD1   | 2.47                     | 0.45              |
| 38:Y:60:VAL:HG22  | 38:Y:66:PHE:CD1   | 2.52                     | 0.45              |
| 40:a:980:A:N7     | 40:a:1136:G:H5'   | 2.32                     | 0.45              |
| 40:a:1182:G:H2'   | 40:a:1183:U:O4'   | 2.17                     | 0.45              |
| 40:a:1398:C:C2    | 40:a:1399:C:C5    | 3.04                     | 0.45              |
| 40:a:1441:G:H2'   | 40:a:1442:U:H6    | 1.82                     | 0.45              |
| 40:a:2646:C:H2'   | 40:a:2647:U:O4'   | 2.17                     | 0.45              |
| 40:a:2747:G:N2    | 40:a:2756:U:C6    | 2.85                     | 0.45              |
| 40:a:2783:U:H2'   | 40:a:2784:U:C6    | 2.52                     | 0.45              |
| 40:a:2839:G:C5    | 40:a:2840:C:C5    | 3.05                     | 0.45              |
| 46:g:30:HIS:CG    | 46:g:31:ASP:N     | 2.85                     | 0.45              |
| 47:h:52:ARG:CD    | 47:h:53:HIS:CE1   | 3.00                     | 0.45              |
| 49:j:172:VAL:HG11 | 49:j:175:LEU:HD11 | 1.99                     | 0.45              |
| 51:l:6:LYS:HZ1    | 51:l:120:VAL:N    | 2.12                     | 0.45              |
| 57:r:127:GLU:OE2  | 57:r:143:ILE:HB   | 2.17                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 58:s:35:ARG:HA     | 58:s:40:HIS:ND1   | 2.32                     | 0.45              |
| 59:t:42:THR:CG2    | 59:t:44:LYS:NZ    | 2.78                     | 0.45              |
| 60:u:55:MET:SD     | 60:u:60:ARG:N     | 2.90                     | 0.45              |
| 62:w:79:LEU:HD23   | 62:w:83:LEU:HD12  | 1.99                     | 0.45              |
| 63:x:86:GLY:HA2    | 63:x:88:LYS:HZ3   | 1.83                     | 0.45              |
| 64:y:14:LYS:NZ     | 64:y:76:THR:O     | 2.49                     | 0.45              |
| 1:0:71:LYS:CG      | 1:0:73:LYS:HE3    | 2.47                     | 0.44              |
| 1:0:74:ILE:HD12    | 1:0:74:ILE:N      | 2.32                     | 0.44              |
| 8:7:11:U:C4'       | 24:K:20:ARG:HH21  | 2.16                     | 0.44              |
| 9:9:23:LEU:O       | 9:9:87:GLU:CD     | 2.60                     | 0.44              |
| 10:A:53:G:N3       | 10:A:54:U:C5      | 2.85                     | 0.44              |
| 11:AA:694:ARG:HH22 | 13:AC:80:GLU:HG3  | 1.82                     | 0.44              |
| 12:AB:6:LEU:HD13   | 14:AE:291:ILE:CG1 | 2.46                     | 0.44              |
| 16:C:70:TYR:C      | 16:C:71:THR:HG23  | 2.42                     | 0.44              |
| 17:D:278:G:OP2     | 35:V:43:LYS:NZ    | 2.49                     | 0.44              |
| 17:D:337:G:H2'     | 17:D:338:A:H8     | 1.80                     | 0.44              |
| 17:D:715:A:H2'     | 17:D:716:A:C8     | 2.52                     | 0.44              |
| 17:D:958:A:C4      | 36:W:55:ARG:HD3   | 2.52                     | 0.44              |
| 17:D:1308:U:H3'    | 37:X:98:ARG:NE    | 2.32                     | 0.44              |
| 17:D:1359:C:OP2    | 32:S:75:ARG:NE    | 2.43                     | 0.44              |
| 17:D:1436:U:H2'    | 17:D:1437:A:H8    | 1.82                     | 0.44              |
| 17:D:1437:A:C2     | 17:D:1438:G:C8    | 3.04                     | 0.44              |
| 17:D:1486:G:H2'    | 17:D:1487:G:O4'   | 2.17                     | 0.44              |
| 22:I:24:ALA:HB3    | 22:I:29:PHE:CD2   | 2.51                     | 0.44              |
| 22:I:72:ARG:HD3    | 22:I:75:ILE:HG22  | 1.99                     | 0.44              |
| 22:I:165:THR:C     | 22:I:166:GLU:OE1  | 2.60                     | 0.44              |
| 33:T:71:LYS:HE2    | 33:T:78:TYR:CD2   | 2.52                     | 0.44              |
| 38:Y:12:VAL:HG22   | 38:Y:54:ILE:O     | 2.17                     | 0.44              |
| 40:a:575:A:C2      | 40:a:576:U:C6     | 3.05                     | 0.44              |
| 40:a:730:A:C2      | 40:a:731:C:C5     | 3.05                     | 0.44              |
| 40:a:730:A:C2      | 40:a:731:C:C6     | 3.05                     | 0.44              |
| 40:a:782:A:N1      | 47:h:225:MET:HE2  | 2.32                     | 0.44              |
| 40:a:1013:C:C2     | 40:a:1014:A:C8    | 3.04                     | 0.44              |
| 40:a:1020:A:C2     | 40:a:1141:U:C2    | 3.06                     | 0.44              |
| 40:a:1310:G:N2     | 40:a:1313:U:C4    | 2.85                     | 0.44              |
| 40:a:1386:C:H2'    | 40:a:1387:A:H8    | 1.81                     | 0.44              |
| 40:a:1792:G:C5'    | 47:h:204:VAL:HG23 | 2.47                     | 0.44              |
| 40:a:2572:A:OP2    | 49:j:149:ASN:O    | 2.35                     | 0.44              |
| 47:h:123:ALA:HB1   | 47:h:125:LYS:CE   | 2.47                     | 0.44              |
| 51:l:23:PHE:CD1    | 51:l:111:GLU:CG   | 3.00                     | 0.44              |
| 54:o:39:LYS:HG2    | 54:o:42:ARG:HH12  | 1.82                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:t:18:ARG:NE     | 59:t:18:ARG:HA     | 2.33                     | 0.44              |
| 1:0:13:ARG:CZ      | 65:z:97:ASP:CG     | 2.91                     | 0.44              |
| 1:0:73:LYS:HZ1     | 1:0:88:GLY:HA3     | 1.82                     | 0.44              |
| 9:9:58:THR:HG23    | 40:a:1108:U:OP1    | 2.17                     | 0.44              |
| 9:9:92:ALA:HB3     | 9:9:129:LEU:HB2    | 1.99                     | 0.44              |
| 10:A:71:C:H2'      | 10:A:72:A:N9       | 2.32                     | 0.44              |
| 10:A:71:C:H2'      | 10:A:72:A:C1'      | 2.47                     | 0.44              |
| 13:AD:192:VAL:HG12 | 13:AD:193:GLU:H    | 1.83                     | 0.44              |
| 14:AE:224:LEU:HD23 | 14:AE:224:LEU:HA   | 1.83                     | 0.44              |
| 17:D:429:U:O2      | 17:D:430:A:N7      | 2.50                     | 0.44              |
| 19:F:26:ALA:CB     | 19:F:28:VAL:HG23   | 2.47                     | 0.44              |
| 21:H:12:SER:O      | 21:H:16:ILE:HG13   | 2.18                     | 0.44              |
| 21:H:308:GLU:C     | 21:H:310:ASP:H     | 2.25                     | 0.44              |
| 21:H:332:VAL:O     | 21:H:333:LEU:HB2   | 2.18                     | 0.44              |
| 22:I:147:LYS:HE2   | 22:I:204:LYS:C     | 2.43                     | 0.44              |
| 24:K:76:LEU:HD12   | 24:K:76:LEU:O      | 2.17                     | 0.44              |
| 25:L:17:GLN:CB     | 25:L:21:MET:HE1    | 2.47                     | 0.44              |
| 25:L:36:ILE:HD12   | 25:L:36:ILE:HA     | 1.82                     | 0.44              |
| 25:L:85:ILE:HG22   | 25:L:86:ARG:HG2    | 1.99                     | 0.44              |
| 33:T:10:LYS:CD     | 33:T:14:GLU:OE2    | 2.65                     | 0.44              |
| 38:Y:33:ASN:OD1    | 38:Y:35:MET:HE2    | 2.17                     | 0.44              |
| 40:a:15:G:O2'      | 48:i:15:MET:HE1    | 2.16                     | 0.44              |
| 40:a:654:A:H61     | 54:o:19:LYS:CD     | 2.31                     | 0.44              |
| 40:a:1349:C:O2     | 40:a:1349:C:H2'    | 2.17                     | 0.44              |
| 40:a:2245:U:O2'    | 40:a:2436:G:OP2    | 2.27                     | 0.44              |
| 40:a:2262:U:OP1    | 40:a:2387:U:O2'    | 2.33                     | 0.44              |
| 40:a:2514:U:H2'    | 40:a:2515:C:H6     | 1.81                     | 0.44              |
| 40:a:2650:U:H2'    | 40:a:2651:C:H6     | 1.81                     | 0.44              |
| 40:a:2747:G:C2     | 40:a:2756:U:C5     | 3.05                     | 0.44              |
| 44:e:13:GLU:C      | 44:e:17:GLU:OE1    | 2.61                     | 0.44              |
| 47:h:265:LYS:HG3   | 47:h:266:PHE:CD2   | 2.52                     | 0.44              |
| 51:l:1:MET:HE3     | 51:l:19:PHE:C      | 2.43                     | 0.44              |
| 60:u:95:LEU:HD12   | 60:u:100:ILE:HG21  | 1.99                     | 0.44              |
| 60:u:101:ILE:HG13  | 60:u:102:GLY:H     | 1.82                     | 0.44              |
| 64:y:31:TRP:CH2    | 64:y:40:LEU:HD11   | 2.52                     | 0.44              |
| 2:1:86:MET:HE1     | 2:1:88:ARG:CD      | 2.42                     | 0.44              |
| 8:7:9:U:OP2        | 8:7:9:U:C6         | 2.71                     | 0.44              |
| 9:9:4:ASN:OD1      | 40:a:1046:A:N7     | 2.50                     | 0.44              |
| 9:9:129:LEU:H      | 9:9:129:LEU:HG     | 1.72                     | 0.44              |
| 10:A:18:G:N2       | 10:A:58:A:N7       | 2.65                     | 0.44              |
| 11:AA:674:ASP:OD2  | 11:AA:1070:HIS:ND1 | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:AC:218:ARG:NH1 | 13:AD:231:PHE:O   | 2.50                     | 0.44              |
| 13:AD:29:GLU:HB3  | 13:AD:200:LYS:HG3 | 1.99                     | 0.44              |
| 10:B:3:C:H2'      | 10:B:4:G:C8       | 2.52                     | 0.44              |
| 10:B:18:G:C5      | 10:B:57:A:N6      | 2.85                     | 0.44              |
| 17:D:153:C:C2     | 17:D:154:U:C5     | 3.06                     | 0.44              |
| 17:D:280:C:O2     | 35:V:40:ARG:NE    | 2.49                     | 0.44              |
| 17:D:309:A:O2'    | 17:D:607:A:N1     | 2.45                     | 0.44              |
| 17:D:414:A:C4     | 17:D:415:A:C8     | 3.05                     | 0.44              |
| 17:D:524:G:H2'    | 17:D:525:C:C6     | 2.52                     | 0.44              |
| 17:D:604:G:H2'    | 17:D:605:U:O4'    | 2.17                     | 0.44              |
| 17:D:675:A:C1'    | 30:Q:118:HIS:CD2  | 2.99                     | 0.44              |
| 17:D:982:U:P      | 32:S:6:MET:HE2    | 2.56                     | 0.44              |
| 17:D:1146:A:C5    | 17:D:1147:C:C5    | 3.06                     | 0.44              |
| 17:D:1436:U:H2'   | 17:D:1437:A:C8    | 2.52                     | 0.44              |
| 20:G:110:SER:OG   | 20:G:113:ARG:NH2  | 2.47                     | 0.44              |
| 21:H:33:LYS:HA    | 21:H:34:ASP:HA    | 1.80                     | 0.44              |
| 21:H:294:VAL:HG11 | 21:H:330:VAL:HG21 | 2.00                     | 0.44              |
| 24:K:12:GLN:HB3   | 24:K:14:LYS:HZ2   | 1.81                     | 0.44              |
| 26:M:106:GLU:O    | 26:M:110:LYS:HG2  | 2.18                     | 0.44              |
| 32:S:6:MET:HE3    | 32:S:63:ARG:HH11  | 1.82                     | 0.44              |
| 32:S:13:ARG:HB3   | 32:S:60:GLN:CG    | 2.46                     | 0.44              |
| 36:W:79:THR:HG23  | 36:W:79:THR:O     | 2.18                     | 0.44              |
| 38:Y:14:ALA:O     | 38:Y:16:MET:N     | 2.51                     | 0.44              |
| 40:a:66:C:N4      | 40:a:74:A:N6      | 2.66                     | 0.44              |
| 40:a:152:A:H2'    | 40:a:153:U:H6     | 1.82                     | 0.44              |
| 40:a:564:C:H1'    | 65:z:37:GLN:NE2   | 2.32                     | 0.44              |
| 40:a:597:G:H2'    | 40:a:598:U:C6     | 2.52                     | 0.44              |
| 40:a:966:G:O4'    | 40:a:2267:A:N6    | 2.51                     | 0.44              |
| 40:a:2345:G:N3    | 40:a:2381:A:H2'   | 2.33                     | 0.44              |
| 40:a:2347:C:C2    | 40:a:2348:U:C5    | 3.05                     | 0.44              |
| 45:f:41:THR:C     | 45:f:45:ARG:NH2   | 2.75                     | 0.44              |
| 47:h:146:MET:HE2  | 47:h:153:GLN:OE1  | 2.17                     | 0.44              |
| 53:n:10:ASP:OD1   | 53:n:11:GLU:HG3   | 2.17                     | 0.44              |
| 55:p:69:ARG:NH1   | 55:p:73:ASN:ND2   | 2.66                     | 0.44              |
| 55:p:141:ILE:HG13 | 55:p:142:GLY:N    | 2.32                     | 0.44              |
| 62:w:87:PHE:HE2   | 62:w:115:LEU:HD11 | 1.83                     | 0.44              |
| 62:w:98:LEU:N     | 62:w:112:TYR:O    | 2.51                     | 0.44              |
| 63:x:88:LYS:O     | 63:x:115:LEU:HD12 | 2.16                     | 0.44              |
| 1:0:73:LYS:HD3    | 1:0:86:GLN:HE21   | 1.82                     | 0.44              |
| 9:9:19:ALA:CB     | 9:9:69:PHE:HE2    | 2.31                     | 0.44              |
| 12:AB:16:ARG:C    | 12:AB:19:GLU:H    | 2.25                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:AB:38:ILE:HA   | 12:AB:42:LYS:O    | 2.18                     | 0.44              |
| 14:AE:708:ASN:OD1 | 14:AE:708:ASN:N   | 2.50                     | 0.44              |
| 14:AE:802:ASP:OD1 | 14:AE:1348:LYS:NZ | 2.42                     | 0.44              |
| 10:B:18:G:N7      | 10:B:57:A:N6      | 2.65                     | 0.44              |
| 16:C:41:PRO:HD2   | 21:H:339:ARG:CZ   | 2.47                     | 0.44              |
| 17:D:33:A:H2'     | 17:D:34:C:C6      | 2.53                     | 0.44              |
| 17:D:198:G:OP2    | 17:D:198:G:C8     | 2.70                     | 0.44              |
| 17:D:753:A:OP1    | 33:T:73:LYS:NZ    | 2.50                     | 0.44              |
| 17:D:1250:A:H2'   | 17:D:1251:A:C8    | 2.52                     | 0.44              |
| 17:D:1408:A:H2'   | 17:D:1409:C:C6    | 2.53                     | 0.44              |
| 18:E:25:ARG:O     | 18:E:28:MET:HB2   | 2.18                     | 0.44              |
| 18:E:49:LYS:O     | 18:E:53:GLU:HG2   | 2.16                     | 0.44              |
| 20:G:52:GLU:C     | 20:G:56:GLU:OE1   | 2.60                     | 0.44              |
| 20:G:100:MET:SD   | 20:G:101:LEU:HD23 | 2.56                     | 0.44              |
| 21:H:297:GLU:OE1  | 21:H:297:GLU:N    | 2.49                     | 0.44              |
| 21:H:332:VAL:O    | 21:H:344:LEU:HA   | 2.17                     | 0.44              |
| 24:K:50:TYR:C     | 24:K:66:LYS:HE3   | 2.43                     | 0.44              |
| 28:O:86:ALA:C     | 28:O:89:GLU:HG2   | 2.43                     | 0.44              |
| 29:P:40:ILE:HD12  | 29:P:73:LEU:CD2   | 2.48                     | 0.44              |
| 30:Q:52:PHE:CE1   | 30:Q:65:VAL:HG21  | 2.52                     | 0.44              |
| 36:W:5:LEU:HD12   | 36:W:6:LYS:N      | 2.32                     | 0.44              |
| 36:W:39:THR:HG22  | 36:W:40:ILE:N     | 2.33                     | 0.44              |
| 40:a:65:U:N3      | 40:a:66:C:C5      | 2.86                     | 0.44              |
| 40:a:607:U:C6     | 40:a:620:G:N7     | 2.85                     | 0.44              |
| 40:a:677:A:O2'    | 40:a:2071:A:H5'   | 2.18                     | 0.44              |
| 40:a:1064:C:O2'   | 40:a:1065:U:C6    | 2.62                     | 0.44              |
| 40:a:1144:A:C4    | 40:a:1145:C:C5    | 3.05                     | 0.44              |
| 40:a:1146:C:C2    | 40:a:1147:A:C8    | 3.05                     | 0.44              |
| 40:a:1442:U:H2'   | 40:a:1443:U:H6    | 1.79                     | 0.44              |
| 40:a:2021:C:OP1   | 48:i:9:THR:HG21   | 2.18                     | 0.44              |
| 40:a:2098:U:H2'   | 40:a:2099:U:O4'   | 2.18                     | 0.44              |
| 40:a:2298:A:P     | 53:n:72:LYS:HZ3   | 2.36                     | 0.44              |
| 40:a:2314:A:P     | 53:n:88:LYS:HZ2   | 2.39                     | 0.44              |
| 40:a:2492:U:C2'   | 40:a:2493:U:H5'   | 2.48                     | 0.44              |
| 42:c:41:GLU:O     | 42:c:44:LYS:HD2   | 2.16                     | 0.44              |
| 42:c:43:GLU:OE1   | 42:c:45:ARG:CB    | 2.65                     | 0.44              |
| 45:f:4:THR:CG2    | 45:f:37:GLU:OE2   | 2.65                     | 0.44              |
| 47:h:164:ILE:O    | 47:h:164:ILE:CG2  | 2.65                     | 0.44              |
| 47:h:240:PHE:CD2  | 47:h:240:PHE:O    | 2.71                     | 0.44              |
| 47:h:251:GLN:OE1  | 47:h:255:LYS:CB   | 2.65                     | 0.44              |
| 51:l:23:PHE:CE2   | 51:l:25:GLU:HB2   | 2.52                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:n:117:LEU:N    | 53:n:177:PHE:O     | 2.51                     | 0.44              |
| 54:o:31:HIS:C     | 54:o:33:LEU:HG     | 2.42                     | 0.44              |
| 54:o:55:LEU:C     | 54:o:55:LEU:HD23   | 2.42                     | 0.44              |
| 58:s:31:GLU:HG2   | 58:s:142:ILE:HG23  | 1.98                     | 0.44              |
| 61:v:104:GLU:OE1  | 61:v:104:GLU:HA    | 2.17                     | 0.44              |
| 4:3:6:ARG:CG      | 4:3:7:ARG:H        | 2.31                     | 0.44              |
| 4:3:49:VAL:HG23   | 4:3:51:ALA:O       | 2.16                     | 0.44              |
| 9:9:59:LEU:HD22   | 9:9:62:ARG:HE      | 1.81                     | 0.44              |
| 10:A:72:A:C3'     | 10:A:73:A:H5''     | 2.47                     | 0.44              |
| 11:AA:560:PRO:HB2 | 14:AE:776:THR:HG21 | 2.00                     | 0.44              |
| 11:AA:998:LEU:HG  | 11:AA:1011:LEU:HB3 | 1.99                     | 0.44              |
| 12:AB:17:ALA:O    | 12:AB:20:HIS:HB2   | 2.17                     | 0.44              |
| 10:B:18:G:N2      | 10:B:58:A:N7       | 2.65                     | 0.44              |
| 16:C:70:TYR:CE2   | 25:L:49:TYR:CE1    | 3.05                     | 0.44              |
| 17:D:375:U:OP2    | 34:U:70:ARG:NE     | 2.51                     | 0.44              |
| 17:D:598:U:C2     | 17:D:599:C:C5      | 3.06                     | 0.44              |
| 17:D:735:C:C2     | 17:D:736:C:C5      | 3.05                     | 0.44              |
| 17:D:1333:A:H2'   | 17:D:1334:G:O4'    | 2.17                     | 0.44              |
| 18:E:16:LYS:HG3   | 18:E:19:LYS:HE3    | 1.98                     | 0.44              |
| 18:E:58:VAL:HG12  | 18:E:72:ALA:HB1    | 1.99                     | 0.44              |
| 20:G:64:LYS:HE2   | 20:G:64:LYS:HA     | 1.99                     | 0.44              |
| 20:G:163:VAL:CG1  | 20:G:185:ALA:HA    | 2.47                     | 0.44              |
| 20:G:171:ILE:H    | 20:G:171:ILE:HD12  | 1.82                     | 0.44              |
| 21:H:53:PHE:HE1   | 21:H:68:VAL:HG21   | 1.82                     | 0.44              |
| 23:J:172:GLU:CD   | 23:J:183:LYS:HD2   | 2.42                     | 0.44              |
| 25:L:78:PHE:HD1   | 25:L:87:SER:HB3    | 1.82                     | 0.44              |
| 28:O:91:ASP:HB3   | 28:O:94:LEU:HG     | 1.99                     | 0.44              |
| 28:O:113:ARG:HG3  | 28:O:115:LYS:HZ2   | 1.83                     | 0.44              |
| 29:P:24:GLU:OE2   | 29:P:92:LEU:CD2    | 2.66                     | 0.44              |
| 31:R:38:TYR:CE2   | 31:R:40:THR:CG2    | 3.01                     | 0.44              |
| 32:S:47:LYS:O     | 32:S:50:THR:OG1    | 2.25                     | 0.44              |
| 33:T:3:LEU:CD2    | 33:T:8:THR:HG23    | 2.47                     | 0.44              |
| 33:T:11:ILE:HD11  | 33:T:30:ALA:HB1    | 1.99                     | 0.44              |
| 38:Y:15:GLY:CA    | 38:Y:50:LYS:HG3    | 2.40                     | 0.44              |
| 40:a:479:A:H4'    | 40:a:480:A:OP1     | 2.18                     | 0.44              |
| 40:a:536:G:H4'    | 65:z:57:PHE:CZ     | 2.53                     | 0.44              |
| 40:a:1021:A:C2    | 40:a:1141:U:O4     | 2.70                     | 0.44              |
| 40:a:1084:A:N6    | 40:a:1085:A:N1     | 2.66                     | 0.44              |
| 40:a:1250:G:OP2   | 60:u:21:ARG:NE     | 2.47                     | 0.44              |
| 40:a:1434:A:H2'   | 40:a:1435:G:C8     | 2.53                     | 0.44              |
| 40:a:1656:C:C2    | 40:a:1657:U:C5     | 3.05                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:a:2175:C:C2'    | 40:a:2176:A:C8    | 3.00                     | 0.44              |
| 40:a:2450:A:C2     | 40:a:2451:A:C4    | 3.06                     | 0.44              |
| 40:a:2718:G:O2'    | 40:a:2847:U:H5''  | 2.18                     | 0.44              |
| 47:h:220:VAL:HG23  | 47:h:225:MET:HE3  | 2.00                     | 0.44              |
| 51:l:90:GLN:OE1    | 51:l:92:HIS:CD2   | 2.70                     | 0.44              |
| 51:l:117:ARG:NH1   | 60:u:1:MET:HE2    | 2.32                     | 0.44              |
| 51:l:147:LEU:HB2   | 51:l:183:PHE:CD2  | 2.48                     | 0.44              |
| 53:n:175:PHE:CG    | 53:n:176:PRO:HD2  | 2.52                     | 0.44              |
| 58:s:28:LEU:HD12   | 58:s:142:ILE:CG2  | 2.47                     | 0.44              |
| 58:s:124:VAL:O     | 58:s:125:TYR:HD1  | 2.01                     | 0.44              |
| 58:s:132:HIS:HA    | 58:s:135:GLN:OE1  | 2.17                     | 0.44              |
| 5:4:55:GLU:OE1     | 5:4:55:GLU:N      | 2.42                     | 0.44              |
| 9:9:138:ARG:NH1    | 39:Z:10:ALA:O     | 2.51                     | 0.44              |
| 11:AA:24:VAL:HG11  | 11:AA:704:MET:HE1 | 1.98                     | 0.44              |
| 12:AB:141:LEU:CA   | 12:AB:153:SER:N   | 2.75                     | 0.44              |
| 12:AB:141:LEU:HD23 | 12:AB:143:LEU:HG  | 1.98                     | 0.44              |
| 10:B:11:A:H2'      | 10:B:12:G:O4'     | 2.17                     | 0.44              |
| 10:B:71:C:H2'      | 10:B:72:A:C1'     | 2.47                     | 0.44              |
| 10:B:71:C:C3'      | 10:B:72:A:C8      | 2.99                     | 0.44              |
| 16:C:34:THR:OG1    | 16:C:38:LYS:HB2   | 2.17                     | 0.44              |
| 16:C:40:VAL:HG22   | 21:H:339:ARG:HE   | 1.83                     | 0.44              |
| 17:D:284:C:C2      | 17:D:285:C:C5     | 3.06                     | 0.44              |
| 17:D:564:C:OP1     | 31:R:12:ARG:CZ    | 2.66                     | 0.44              |
| 17:D:704:A:C4      | 17:D:705:G:C8     | 3.06                     | 0.44              |
| 17:D:1062:U:H2'    | 17:D:1063:C:C6    | 2.53                     | 0.44              |
| 20:G:96:TRP:CZ2    | 20:G:100:MET:HE3  | 2.52                     | 0.44              |
| 21:H:19:ARG:O      | 21:H:72:LEU:HD13  | 2.18                     | 0.44              |
| 21:H:76:GLU:OE1    | 21:H:79:PHE:HA    | 2.17                     | 0.44              |
| 22:I:152:GLU:OE2   | 22:I:165:THR:HG23 | 2.18                     | 0.44              |
| 23:J:69:GLU:HA     | 23:J:72:PHE:HD2   | 1.83                     | 0.44              |
| 24:K:50:TYR:O      | 24:K:66:LYS:HE3   | 2.17                     | 0.44              |
| 25:L:5:GLU:CD      | 25:L:61:LEU:HD11  | 2.42                     | 0.44              |
| 28:O:89:GLU:HG3    | 28:O:90:TYR:N     | 2.33                     | 0.44              |
| 29:P:66:GLU:HG3    | 32:S:99:ALA:HB2   | 2.00                     | 0.44              |
| 29:P:73:LEU:C      | 29:P:73:LEU:HD23  | 2.42                     | 0.44              |
| 33:T:26:GLU:HG3    | 33:T:27:VAL:N     | 2.33                     | 0.44              |
| 33:T:76:ALA:C      | 33:T:80:GLN:NE2   | 2.68                     | 0.44              |
| 37:X:106:ALA:HB3   | 37:X:110:LYS:CD   | 2.48                     | 0.44              |
| 38:Y:82:ALA:HB3    | 38:Y:108:ILE:CD1  | 2.48                     | 0.44              |
| 40:a:145:C:H2'     | 40:a:146:A:C8     | 2.53                     | 0.44              |
| 40:a:208:C:H2'     | 40:a:209:C:C6     | 2.53                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 40:a:861:A:H2'    | 40:a:862:G:O4'   | 2.17                     | 0.44              |
| 40:a:1342:A:O2'   | 40:a:1344:U:OP2  | 2.31                     | 0.44              |
| 40:a:1432:G:H2'   | 40:a:1433:A:H8   | 1.80                     | 0.44              |
| 40:a:1824:G:P     | 47:h:52:ARG:CZ   | 3.06                     | 0.44              |
| 40:a:2063:C:N3    | 40:a:2064:C:C5   | 2.86                     | 0.44              |
| 40:a:2093:G:P     | 57:r:22:LYS:HG2  | 2.58                     | 0.44              |
| 40:a:2297:A:C2    | 40:a:2320:U:C1'  | 3.00                     | 0.44              |
| 40:a:2484:G:OP1   | 61:v:44:ARG:HD2  | 2.18                     | 0.44              |
| 40:a:2616:C:C2    | 40:a:2617:U:C6   | 3.06                     | 0.44              |
| 47:h:74:ILE:HB    | 47:h:96:TYR:CD1  | 2.53                     | 0.44              |
| 49:j:81:GLU:O     | 49:j:82:PHE:HD1  | 2.01                     | 0.44              |
| 62:w:60:VAL:HA    | 62:w:63:ARG:CZ   | 2.48                     | 0.44              |
| 1:0:60:LYS:N      | 1:0:60:LYS:HD3   | 2.33                     | 0.44              |
| 10:A:18:G:C5      | 10:A:57:A:N6     | 2.85                     | 0.44              |
| 10:A:18:G:N7      | 10:A:57:A:N6     | 2.65                     | 0.44              |
| 14:AE:288:PRO:HD2 | 14:AE:291:ILE:CB | 2.42                     | 0.44              |
| 10:B:75:C:P       | 40:a:2602:A:C2'  | 3.05                     | 0.44              |
| 16:C:18:VAL:HG13  | 16:C:51:TYR:HE1  | 1.83                     | 0.44              |
| 17:D:262:A:H2'    | 17:D:263:A:C8    | 2.53                     | 0.44              |
| 17:D:360:G:H2'    | 17:D:361:G:C8    | 2.53                     | 0.44              |
| 17:D:642:A:C5     | 17:D:643:C:C5    | 3.06                     | 0.44              |
| 17:D:1160:G:C6    | 17:D:1161:C:C5   | 3.06                     | 0.44              |
| 17:D:1434:A:H2'   | 17:D:1435:G:O4'  | 2.18                     | 0.44              |
| 21:H:5:PHE:CZ     | 21:H:9:PHE:CE1   | 3.06                     | 0.44              |
| 30:Q:21:ALA:HB3   | 30:Q:84:VAL:HG22 | 1.99                     | 0.44              |
| 30:Q:91:PRO:HD2   | 30:Q:92:GLY:H    | 1.83                     | 0.44              |
| 31:R:18:LYS:HD3   | 31:R:19:SER:N    | 2.33                     | 0.44              |
| 31:R:25:GLU:OE2   | 31:R:30:LYS:HE3  | 2.18                     | 0.44              |
| 32:S:87:ALA:CA    | 32:S:90:ARG:CZ   | 2.96                     | 0.44              |
| 35:V:27:ARG:HH22  | 35:V:42:THR:N    | 2.16                     | 0.44              |
| 35:V:30:LYS:HB2   | 35:V:37:PHE:CE1  | 2.52                     | 0.44              |
| 38:Y:44:LYS:HG2   | 38:Y:68:PHE:HE2  | 1.83                     | 0.44              |
| 40:a:27:G:C4      | 40:a:512:G:N2    | 2.86                     | 0.44              |
| 40:a:30:G:H2'     | 40:a:31:C:H6     | 1.81                     | 0.44              |
| 40:a:153:U:H2'    | 40:a:154:U:C6    | 2.53                     | 0.44              |
| 40:a:580:U:O3'    | 65:z:31:VAL:HG13 | 2.17                     | 0.44              |
| 40:a:910:A:H8     | 61:v:12:MET:CE   | 2.31                     | 0.44              |
| 40:a:957:C:H5'    | 61:v:75:GLU:OE1  | 2.18                     | 0.44              |
| 40:a:1414:C:H2'   | 40:a:1415:U:C6   | 2.52                     | 0.44              |
| 40:a:1863:G:H2'   | 40:a:1864:U:H6   | 1.83                     | 0.44              |
| 40:a:1936:A:C8    | 40:a:1945:G:N7   | 2.86                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:a:1997:C:OP1    | 49:j:128:ARG:NH1  | 2.50                     | 0.44              |
| 42:c:33:LEU:O      | 42:c:34:HIS:CG    | 2.70                     | 0.44              |
| 45:f:41:THR:O      | 45:f:43:ALA:N     | 2.51                     | 0.44              |
| 47:h:200:HIS:O     | 47:h:203:ARG:HG2  | 2.17                     | 0.44              |
| 49:j:204:LYS:HD3   | 49:j:205:PRO:HD2  | 2.00                     | 0.44              |
| 55:p:27:LYS:HG2    | 55:p:32:GLU:HG3   | 2.00                     | 0.44              |
| 55:p:83:PHE:HB2    | 55:p:141:ILE:HD13 | 2.00                     | 0.44              |
| 61:v:3:GLN:OE1     | 61:v:4:PRO:O      | 2.35                     | 0.44              |
| 62:w:13:ASN:O      | 62:w:17:ARG:HG3   | 2.17                     | 0.44              |
| 64:y:7:GLN:HE21    | 64:y:10:GLN:HE21  | 1.65                     | 0.44              |
| 6:5:11:DA:C5'      | 12:AB:67:THR:O    | 2.66                     | 0.44              |
| 8:7:12:U:C3'       | 8:7:12:U:C6       | 3.00                     | 0.44              |
| 13:AD:31:LEU:HD21  | 13:AD:39:LEU:HD12 | 2.00                     | 0.44              |
| 14:AE:117:LEU:HG   | 14:AE:118:LYS:HG3 | 2.00                     | 0.44              |
| 14:AE:975:ILE:HG22 | 14:AE:977:SER:H   | 1.83                     | 0.44              |
| 16:C:29:LEU:CD2    | 16:C:59:ILE:HD13  | 2.48                     | 0.44              |
| 17:D:323:U:H4'     | 18:E:17:ALA:HB3   | 1.99                     | 0.44              |
| 17:D:376:G:C2      | 17:D:389:A:C2     | 3.06                     | 0.44              |
| 17:D:676:A:H2'     | 17:D:677:U:H6     | 1.82                     | 0.44              |
| 17:D:754:C:O5'     | 33:T:72:ARG:NH1   | 2.51                     | 0.44              |
| 17:D:892:A:H2'     | 17:D:893:C:H6     | 1.83                     | 0.44              |
| 20:G:9:MET:HE1     | 20:G:47:VAL:HG22  | 1.99                     | 0.44              |
| 22:I:156:ARG:CG    | 22:I:193:TYR:HB2  | 2.47                     | 0.44              |
| 23:J:35:GLU:HG2    | 23:J:36:GLN:N     | 2.32                     | 0.44              |
| 23:J:49:SER:O      | 23:J:53:VAL:HG13  | 2.18                     | 0.44              |
| 27:N:35:ALA:HB1    | 27:N:110:VAL:HG11 | 1.99                     | 0.44              |
| 30:Q:51:GLY:O      | 30:Q:56:ARG:NH1   | 2.50                     | 0.44              |
| 31:R:30:LYS:C      | 31:R:81:LEU:HD12  | 2.42                     | 0.44              |
| 31:R:74:LEU:HD11   | 31:R:80:ILE:CG1   | 2.48                     | 0.44              |
| 32:S:20:TYR:CD2    | 32:S:55:SER:OG    | 2.67                     | 0.44              |
| 33:T:63:ARG:HD2    | 33:T:67:LEU:HD21  | 2.00                     | 0.44              |
| 40:a:128:C:C2      | 40:a:129:C:C5     | 3.06                     | 0.44              |
| 40:a:536:G:H4'     | 65:z:57:PHE:HZ    | 1.82                     | 0.44              |
| 40:a:594:U:C2      | 40:a:595:C:C5     | 3.05                     | 0.44              |
| 40:a:1007:C:H5''   | 58:s:37:ARG:NE    | 2.31                     | 0.44              |
| 40:a:1839:G:C4     | 40:a:1840:G:C8    | 3.06                     | 0.44              |
| 40:a:2175:C:H2'    | 40:a:2176:A:N7    | 2.33                     | 0.44              |
| 40:a:2548:U:C2     | 40:a:2549:G:C8    | 3.06                     | 0.44              |
| 44:e:59:GLU:CD     | 44:e:60:LYS:N     | 2.76                     | 0.44              |
| 45:f:31:ARG:HG2    | 45:f:34:HIS:HB2   | 2.00                     | 0.44              |
| 49:j:61:THR:OG1    | 49:j:63:PRO:HD2   | 2.18                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:k:7:GLU:HG3    | 50:k:27:LYS:HZ3    | 1.83                     | 0.44              |
| 51:l:198:GLU:OE1  | 51:l:198:GLU:N     | 2.43                     | 0.44              |
| 53:n:15:LYS:O     | 53:n:19:GLU:OE1    | 2.35                     | 0.44              |
| 54:o:30:ARG:HH12  | 60:u:62:PRO:N      | 2.15                     | 0.44              |
| 54:o:45:ARG:HB3   | 54:o:46:PRO:CD     | 2.48                     | 0.44              |
| 58:s:98:GLU:O     | 58:s:100:VAL:N     | 2.51                     | 0.44              |
| 59:t:44:LYS:N     | 59:t:44:LYS:HD2    | 2.33                     | 0.44              |
| 59:t:48:PRO:HB2   | 59:t:49:ARG:HE     | 1.81                     | 0.44              |
| 61:v:38:ARG:HB2   | 61:v:98:PRO:HD3    | 2.00                     | 0.44              |
| 63:x:50:ALA:O     | 63:x:81:ARG:NH2    | 2.51                     | 0.44              |
| 2:1:36:LEU:N      | 2:1:36:LEU:HD12    | 2.33                     | 0.44              |
| 4:3:7:ARG:NH2     | 40:a:84:A:O2'      | 2.51                     | 0.44              |
| 6:5:18:DG:C4      | 6:5:19:DC:C5       | 3.06                     | 0.44              |
| 6:5:20:DC:H1'     | 6:5:21:DA:H5'      | 2.00                     | 0.44              |
| 8:7:4:U:C5        | 17:D:1403:C:H1'    | 2.52                     | 0.44              |
| 9:9:6:GLN:CA      | 9:9:9:GLN:HE22     | 2.30                     | 0.44              |
| 10:A:19:G:O6      | 40:a:2111:U:H3'    | 2.18                     | 0.44              |
| 11:AA:811:ASN:ND2 | 11:AA:1098:LEU:O   | 2.51                     | 0.44              |
| 12:AB:31:PRO:C    | 12:AB:50:LEU:H     | 2.22                     | 0.44              |
| 12:AB:31:PRO:HG2  | 12:AB:51:PHE:CE2   | 2.53                     | 0.44              |
| 13:AD:83:LEU:HD11 | 14:AE:526:VAL:HB   | 1.99                     | 0.44              |
| 14:AE:658:GLU:HA  | 14:AE:661:VAL:HG22 | 2.00                     | 0.44              |
| 17:D:219:U:C2     | 17:D:220:G:C8      | 3.05                     | 0.44              |
| 17:D:404:G:N7     | 23:J:2:ALA:HB3     | 2.33                     | 0.44              |
| 17:D:621:A:H2'    | 17:D:622:A:C8      | 2.53                     | 0.44              |
| 17:D:622:A:C8     | 17:D:623:C:C5      | 3.06                     | 0.44              |
| 17:D:1120:C:H2'   | 17:D:1121:U:H6     | 1.83                     | 0.44              |
| 18:E:21:ASN:HB3   | 18:E:25:ARG:CZ     | 2.48                     | 0.44              |
| 18:E:78:ASN:O     | 18:E:82:GLN:CD     | 2.61                     | 0.44              |
| 20:G:48:PRO:O     | 20:G:52:GLU:HG2    | 2.18                     | 0.44              |
| 21:H:8:LEU:HD12   | 21:H:11:GLU:OE2    | 2.18                     | 0.44              |
| 22:I:157:LEU:CD1  | 22:I:166:GLU:OE1   | 2.66                     | 0.44              |
| 25:L:9:MET:HE3    | 25:L:9:MET:HB3     | 1.85                     | 0.44              |
| 27:N:35:ALA:HB1   | 27:N:110:VAL:CG1   | 2.48                     | 0.44              |
| 28:O:94:LEU:O     | 28:O:97:GLU:CD     | 2.60                     | 0.44              |
| 30:Q:84:VAL:HG21  | 30:Q:97:ILE:HD11   | 1.99                     | 0.44              |
| 31:R:24:LEU:HD23  | 31:R:95:TYR:HE1    | 1.83                     | 0.44              |
| 36:W:62:VAL:HG13  | 36:W:66:MET:CE     | 2.44                     | 0.44              |
| 38:Y:19:PRO:CG    | 38:Y:23:VAL:CG2    | 2.95                     | 0.44              |
| 40:a:30:G:O2'     | 40:a:1214:A:N3     | 2.49                     | 0.44              |
| 40:a:221:A:C4     | 40:a:266:G:N7      | 2.85                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 40:a:234:U:C4      | 40:a:235:U:C5       | 3.06                     | 0.44              |
| 40:a:579:G:H2'     | 40:a:580:U:C6       | 2.53                     | 0.44              |
| 40:a:1360:G:C8     | 40:a:1361:G:C8      | 3.06                     | 0.44              |
| 40:a:1996:C:OP1    | 59:t:31:ARG:NH2     | 2.51                     | 0.44              |
| 40:a:2617:U:C2     | 40:a:2618:G:C8      | 3.06                     | 0.44              |
| 43:d:45:A:C4       | 43:d:46:A:C8        | 3.05                     | 0.44              |
| 43:d:69:G:C5       | 43:d:70:C:C6        | 3.06                     | 0.44              |
| 48:i:17:ARG:CA     | 48:i:20:ASP:OD1     | 2.66                     | 0.44              |
| 49:j:104:VAL:HG12  | 49:j:105:LYS:N      | 2.33                     | 0.44              |
| 49:j:131:ASP:OD1   | 49:j:133:THR:O      | 2.36                     | 0.44              |
| 51:l:6:LYS:CE      | 51:l:119:ILE:CG2    | 2.94                     | 0.44              |
| 53:n:6:ASP:O       | 53:n:10:ASP:OD2     | 2.36                     | 0.44              |
| 54:o:45:ARG:HD2    | 54:o:45:ARG:C       | 2.43                     | 0.44              |
| 55:p:8:PRO:C       | 55:p:69:ARG:NH2     | 2.75                     | 0.44              |
| 55:p:121:ILE:HD12  | 55:p:141:ILE:CG2    | 2.40                     | 0.44              |
| 56:q:3:VAL:HG12    | 56:q:36:ARG:HB3     | 2.00                     | 0.44              |
| 65:z:14:HIS:O      | 65:z:18:LEU:HD23    | 2.18                     | 0.44              |
| 2:1:19:LEU:HD23    | 2:1:19:LEU:C        | 2.43                     | 0.43              |
| 2:1:36:LEU:HD23    | 2:1:48:LYS:CA       | 2.48                     | 0.43              |
| 9:9:129:LEU:CD1    | 9:9:130:PRO:HD3     | 2.45                     | 0.43              |
| 10:A:3:C:H2'       | 10:A:4:G:C8         | 2.53                     | 0.43              |
| 10:A:11:A:H2'      | 10:A:12:G:O4'       | 2.17                     | 0.43              |
| 11:AA:1157:GLN:HG3 | 11:AA:1159:VAL:HG13 | 2.00                     | 0.43              |
| 14:AE:74:LYS:HZ3   | 29:P:89:ARG:HG2     | 1.83                     | 0.43              |
| 17:D:108:G:H5''    | 17:D:108:G:N3       | 2.33                     | 0.43              |
| 17:D:235:C:H2'     | 17:D:236:A:H8       | 1.83                     | 0.43              |
| 17:D:415:A:C6      | 17:D:416:G:C5       | 3.05                     | 0.43              |
| 17:D:610:U:C2      | 17:D:611:C:C6       | 3.06                     | 0.43              |
| 17:D:736:C:H4'     | 25:L:88:MET:HE2     | 1.99                     | 0.43              |
| 17:D:824:G:C6      | 17:D:877:G:C6       | 3.05                     | 0.43              |
| 17:D:877:G:H5''    | 27:N:80:ARG:CD      | 2.49                     | 0.43              |
| 17:D:1240:U:H5     | 26:M:116:MET:HE2    | 1.83                     | 0.43              |
| 22:I:112:ASP:O     | 22:I:116:VAL:HG23   | 2.18                     | 0.43              |
| 27:N:110:VAL:O     | 27:N:111:MET:SD     | 2.75                     | 0.43              |
| 28:O:56:ASP:OD1    | 28:O:56:ASP:N       | 2.51                     | 0.43              |
| 29:P:45:ARG:HD3    | 29:P:47:GLU:OE2     | 2.18                     | 0.43              |
| 30:Q:63:ALA:CB     | 30:Q:92:GLY:HA3     | 2.48                     | 0.43              |
| 34:U:8:ARG:H       | 34:U:28:ARG:HD3     | 1.81                     | 0.43              |
| 40:a:6:A:O2'       | 58:s:132:HIS:ND1    | 2.50                     | 0.43              |
| 40:a:400:G:OP2     | 42:c:57:ARG:NH1     | 2.46                     | 0.43              |
| 40:a:2016:U:H2'    | 40:a:2017:U:C6      | 2.52                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:a:2025:C:H2'   | 40:a:2026:U:C6    | 2.53                     | 0.43              |
| 40:a:2305:U:H5''  | 53:n:131:GLY:HA3  | 2.00                     | 0.43              |
| 40:a:2387:U:C4'   | 41:b:41:ARG:NH1   | 2.81                     | 0.43              |
| 40:a:2806:C:H2'   | 40:a:2807:U:O4'   | 2.18                     | 0.43              |
| 47:h:108:LYS:HZ3  | 47:h:194:GLU:H    | 1.64                     | 0.43              |
| 48:i:23:THR:O     | 48:i:23:THR:HG23  | 2.17                     | 0.43              |
| 52:m:41:ARG:NE    | 52:m:41:ARG:HA    | 2.33                     | 0.43              |
| 53:n:63:GLN:HG3   | 53:n:95:ARG:HD3   | 1.99                     | 0.43              |
| 54:o:8:ARG:HA     | 54:o:8:ARG:HE     | 1.82                     | 0.43              |
| 65:z:66:ASN:CG    | 65:z:76:TYR:HB2   | 2.42                     | 0.43              |
| 1:0:77:PHE:CD2    | 65:z:40:ILE:HG21  | 2.53                     | 0.43              |
| 3:2:56:GLU:CD     | 3:2:88:LYS:N      | 2.76                     | 0.43              |
| 4:3:7:ARG:HG3     | 4:3:8:ASP:N       | 2.33                     | 0.43              |
| 10:A:32:C:O3'     | 26:M:86:GLN:NE2   | 2.51                     | 0.43              |
| 12:AB:130:PHE:HB3 | 12:AB:133:PRO:HD3 | 2.00                     | 0.43              |
| 10:B:75:C:OP1     | 40:a:2602:A:C8    | 2.72                     | 0.43              |
| 17:D:746:A:H2'    | 17:D:747:A:C8     | 2.53                     | 0.43              |
| 17:D:1325:C:N3    | 17:D:1326:U:C5    | 2.86                     | 0.43              |
| 19:F:32:VAL:HG11  | 30:Q:89:PRO:HG3   | 1.99                     | 0.43              |
| 20:G:9:MET:HE2    | 20:G:43:LEU:HD22  | 2.00                     | 0.43              |
| 20:G:134:ALA:HA   | 20:G:137:ARG:HE   | 1.83                     | 0.43              |
| 21:H:49:PRO:HD3   | 21:H:84:LEU:HD21  | 1.99                     | 0.43              |
| 22:I:34:ASP:HB2   | 32:S:65:ARG:CZ    | 2.48                     | 0.43              |
| 22:I:54:ARG:NH1   | 22:I:69:HIS:NE2   | 2.66                     | 0.43              |
| 22:I:55:ILE:HD12  | 22:I:68:ILE:HG12  | 1.99                     | 0.43              |
| 22:I:149:ILE:HG13 | 22:I:201:TRP:O    | 2.18                     | 0.43              |
| 24:K:134:ILE:CG2  | 24:K:135:ASN:N    | 2.81                     | 0.43              |
| 25:L:2:ARG:HB2    | 25:L:4:TYR:CE1    | 2.53                     | 0.43              |
| 27:N:31:LYS:N     | 27:N:31:LYS:HD2   | 2.34                     | 0.43              |
| 27:N:84:ARG:HD2   | 27:N:124:GLU:OE1  | 2.17                     | 0.43              |
| 30:Q:83:GLU:OE1   | 30:Q:83:GLU:N     | 2.51                     | 0.43              |
| 31:R:56:ARG:HG2   | 31:R:62:GLU:CD    | 2.41                     | 0.43              |
| 33:T:32:LEU:HD12  | 33:T:63:ARG:HA    | 1.98                     | 0.43              |
| 37:X:3:ARG:NH2    | 53:n:110:ARG:HD2  | 2.33                     | 0.43              |
| 37:X:71:ARG:NH1   | 37:X:72:GLU:HG3   | 2.33                     | 0.43              |
| 38:Y:99:LYS:CE    | 38:Y:140:GLU:OE2  | 2.67                     | 0.43              |
| 40:a:74:A:N7      | 40:a:88:G:C5      | 2.87                     | 0.43              |
| 40:a:78:U:C5'     | 44:e:4:LYS:NZ     | 2.81                     | 0.43              |
| 40:a:841:G:H2'    | 40:a:842:U:C6     | 2.52                     | 0.43              |
| 40:a:900:A:C5     | 40:a:901:C:C5     | 3.06                     | 0.43              |
| 40:a:1385:A:C4    | 40:a:1403:A:C2    | 3.06                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:a:1657:U:C2     | 40:a:1658:C:C5     | 3.06                     | 0.43              |
| 40:a:2179:C:H2'    | 40:a:2180:U:H6     | 1.84                     | 0.43              |
| 40:a:2846:G:H2'    | 40:a:2847:U:O4'    | 2.18                     | 0.43              |
| 55:p:94:TYR:CE1    | 55:p:152:ARG:CD    | 3.02                     | 0.43              |
| 55:p:149:ARG:HD2   | 55:p:162:VAL:O     | 2.18                     | 0.43              |
| 3:2:56:GLU:OE1     | 3:2:86:THR:C       | 2.61                     | 0.43              |
| 5:4:53:LYS:HB2     | 5:4:56:PHE:HE2     | 1.83                     | 0.43              |
| 8:7:36:A:O3'       | 11:AA:688:GLN:NE2  | 2.51                     | 0.43              |
| 9:9:70:GLU:HG3     | 9:9:71:CYS:N       | 2.34                     | 0.43              |
| 10:A:35:A:H2'      | 10:A:36:U:O4'      | 2.18                     | 0.43              |
| 12:AB:33:ILE:HD11  | 12:AB:104:ILE:HA   | 2.00                     | 0.43              |
| 12:AB:140:MET:C    | 12:AB:152:HIS:C    | 2.85                     | 0.43              |
| 14:AE:283:LEU:HD23 | 14:AE:292:VAL:HG11 | 1.99                     | 0.43              |
| 10:B:72:A:C3'      | 10:B:73:A:H5''     | 2.47                     | 0.43              |
| 17:D:562:U:C3'     | 31:R:14:ARG:NH1    | 2.81                     | 0.43              |
| 17:D:622:A:C8      | 17:D:623:C:C6      | 3.06                     | 0.43              |
| 17:D:678:U:H2'     | 17:D:679:C:C6      | 2.53                     | 0.43              |
| 17:D:1120:C:C2     | 17:D:1121:U:C5     | 3.06                     | 0.43              |
| 17:D:1244:G:C6     | 17:D:1294:G:C6     | 3.06                     | 0.43              |
| 17:D:1317:C:OP2    | 32:S:28:LYS:CE     | 2.67                     | 0.43              |
| 20:G:206:ALA:O     | 20:G:210:VAL:HG23  | 2.18                     | 0.43              |
| 21:H:71:ALA:HB3    | 21:H:83:LEU:O      | 2.18                     | 0.43              |
| 24:K:93:ARG:NH2    | 24:K:93:ARG:CB     | 2.80                     | 0.43              |
| 28:O:21:ILE:CD1    | 28:O:86:ALA:CB     | 2.96                     | 0.43              |
| 28:O:63:LEU:CD1    | 28:O:65:ILE:HD11   | 2.48                     | 0.43              |
| 33:T:10:LYS:CE     | 33:T:10:LYS:HA     | 2.49                     | 0.43              |
| 33:T:10:LYS:HA     | 33:T:10:LYS:HE2    | 2.00                     | 0.43              |
| 35:V:28:PHE:CZ     | 35:V:37:PHE:HB3    | 2.53                     | 0.43              |
| 38:Y:64:ARG:O      | 38:Y:64:ARG:HG3    | 2.17                     | 0.43              |
| 38:Y:102:ARG:NH1   | 38:Y:139:VAL:HG11  | 2.33                     | 0.43              |
| 40:a:66:C:H42      | 40:a:74:A:H62      | 1.67                     | 0.43              |
| 40:a:782:A:C6      | 47:h:225:MET:HE2   | 2.53                     | 0.43              |
| 40:a:963:U:H2'     | 40:a:964:C:C6      | 2.53                     | 0.43              |
| 40:a:1565:C:O2'    | 40:a:1567:G:N7     | 2.47                     | 0.43              |
| 40:a:1820:U:C2     | 47:h:201:MET:HE2   | 2.53                     | 0.43              |
| 40:a:2391:G:P      | 54:o:32:ILE:CD1    | 3.06                     | 0.43              |
| 40:a:2702:G:C4     | 40:a:2703:C:C5     | 3.06                     | 0.43              |
| 43:d:55:U:O2'      | 53:n:26:MET:CE     | 2.67                     | 0.43              |
| 49:j:16:THR:HG23   | 49:j:20:VAL:O      | 2.19                     | 0.43              |
| 49:j:107:VAL:HG13  | 49:j:177:VAL:HG11  | 2.01                     | 0.43              |
| 51:l:23:PHE:CE2    | 51:l:25:GLU:CB     | 3.01                     | 0.43              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 57:r:6:LEU:C      | 57:r:15:LEU:HD13    | 2.43                     | 0.43              |
| 57:r:93:SER:OG    | 57:r:121:VAL:HG13   | 2.18                     | 0.43              |
| 59:t:1:MET:HE1    | 59:t:32:TYR:CB      | 2.49                     | 0.43              |
| 60:u:95:LEU:HD13  | 60:u:100:ILE:HD12   | 2.00                     | 0.43              |
| 61:v:39:GLY:O     | 61:v:96:ILE:N       | 2.33                     | 0.43              |
| 65:z:76:TYR:OH    | 65:z:92:ARG:HG2     | 2.19                     | 0.43              |
| 1:0:93:PHE:CD1    | 1:0:93:PHE:C        | 2.96                     | 0.43              |
| 3:2:6:ARG:NE      | 3:2:42:GLU:CD       | 2.76                     | 0.43              |
| 4:3:4:LYS:O       | 4:3:94:ARG:NH2      | 2.40                     | 0.43              |
| 9:9:3:LEU:CD1     | 9:9:5:LEU:H         | 2.31                     | 0.43              |
| 9:9:18:VAL:HG13   | 9:9:71:CYS:HB2      | 2.00                     | 0.43              |
| 11:AA:11:ILE:HG22 | 11:AA:1172:LEU:HD11 | 1.99                     | 0.43              |
| 12:AB:35:LEU:HA   | 12:AB:106:ASP:OD1   | 2.19                     | 0.43              |
| 12:AB:60:ASP:HA   | 12:AB:61:PRO:HD3    | 1.88                     | 0.43              |
| 10:B:31:G:H5'     | 17:D:1339:A:C2      | 2.54                     | 0.43              |
| 16:C:34:THR:HG22  | 16:C:35:GLU:N       | 2.33                     | 0.43              |
| 17:D:511:C:C2     | 17:D:512:U:C6       | 3.06                     | 0.43              |
| 17:D:633:G:H2'    | 17:D:634:C:H6       | 1.82                     | 0.43              |
| 17:D:882:C:O2'    | 17:D:883:C:H5'      | 2.18                     | 0.43              |
| 17:D:986:U:H2'    | 17:D:987:G:C8       | 2.53                     | 0.43              |
| 17:D:1208:C:C2    | 17:D:1209:C:C6      | 3.07                     | 0.43              |
| 17:D:1437:A:N3    | 17:D:1438:G:C8      | 2.86                     | 0.43              |
| 19:F:51:SER:OG    | 19:F:55:ARG:NH2     | 2.52                     | 0.43              |
| 19:F:66:ARG:NH2   | 19:F:67:ARG:NH2     | 2.66                     | 0.43              |
| 21:H:305:HIS:CG   | 21:H:306:VAL:H      | 2.36                     | 0.43              |
| 24:K:132:ASN:OD1  | 24:K:134:ILE:HG22   | 2.18                     | 0.43              |
| 25:L:18:VAL:HA    | 25:L:21:MET:CE      | 2.47                     | 0.43              |
| 25:L:53:LYS:HD2   | 25:L:53:LYS:O       | 2.18                     | 0.43              |
| 27:N:10:MET:CG    | 27:N:27:MET:HE1     | 2.47                     | 0.43              |
| 30:Q:14:LYS:HD3   | 30:Q:15:GLN:N       | 2.32                     | 0.43              |
| 36:W:12:ASP:OD2   | 36:W:35:SER:CB      | 2.66                     | 0.43              |
| 37:X:64:VAL:O     | 37:X:64:VAL:HG13    | 2.19                     | 0.43              |
| 37:X:90:ARG:NH1   | 37:X:96:PRO:O       | 2.51                     | 0.43              |
| 38:Y:82:ALA:HB3   | 38:Y:108:ILE:HD12   | 2.01                     | 0.43              |
| 40:a:61:C:C2      | 40:a:94:A:C2        | 3.06                     | 0.43              |
| 40:a:250:G:H2'    | 40:a:251:A:C8       | 2.54                     | 0.43              |
| 40:a:598:U:H2'    | 40:a:599:A:H8       | 1.82                     | 0.43              |
| 40:a:1406:U:O2'   | 40:a:1407:G:C5'     | 2.66                     | 0.43              |
| 40:a:1409:U:C2    | 40:a:1410:G:C8      | 3.06                     | 0.43              |
| 40:a:1709:U:H2'   | 40:a:1710:G:H8      | 1.82                     | 0.43              |
| 40:a:1956:U:C2    | 40:a:1957:C:C6      | 3.06                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:a:2216:G:H2'   | 40:a:2217:G:H8     | 1.82                     | 0.43              |
| 40:a:2273:A:H2'   | 40:a:2274:A:C8     | 2.54                     | 0.43              |
| 40:a:2665:A:C2    | 40:a:2666:C:C6     | 3.07                     | 0.43              |
| 40:a:2768:U:OP1   | 58:s:85:LYS:HE3    | 2.19                     | 0.43              |
| 40:a:2884:U:O2    | 48:i:40:ARG:NH2    | 2.51                     | 0.43              |
| 45:f:6:LYS:HD3    | 45:f:6:LYS:N       | 2.33                     | 0.43              |
| 47:h:91:ILE:HG22  | 47:h:92:ALA:N      | 2.33                     | 0.43              |
| 48:i:55:ILE:CD1   | 62:w:112:TYR:CD2   | 3.02                     | 0.43              |
| 51:l:112:LEU:HD23 | 51:l:118:LEU:HD13  | 1.99                     | 0.43              |
| 53:n:126:GLY:HA2  | 53:n:163:ASP:HA    | 2.00                     | 0.43              |
| 57:r:90:LEU:HD21  | 57:r:94:ILE:HD11   | 2.00                     | 0.43              |
| 61:v:112:LEU:HD12 | 61:v:112:LEU:N     | 2.34                     | 0.43              |
| 2:1:1:MET:SD      | 2:1:62:ASP:OD2     | 2.76                     | 0.43              |
| 5:4:31:TYR:HE2    | 43:d:104:A:O4'     | 2.01                     | 0.43              |
| 9:9:23:LEU:HA     | 9:9:118:ILE:HG13   | 2.01                     | 0.43              |
| 10:A:49:G:H8      | 10:A:49:G:O5'      | 2.01                     | 0.43              |
| 12:AB:4:TRP:CE2   | 12:AB:27:ASN:ND2   | 2.87                     | 0.43              |
| 12:AB:37:LYS:HE3  | 12:AB:109:THR:HG21 | 1.99                     | 0.43              |
| 10:B:35:A:H2'     | 10:B:36:U:O4'      | 2.18                     | 0.43              |
| 16:C:54:GLN:HA    | 16:C:57:ARG:NH1    | 2.33                     | 0.43              |
| 21:H:19:ARG:HD3   | 21:H:19:ARG:N      | 2.32                     | 0.43              |
| 21:H:52:GLN:OE1   | 21:H:52:GLN:HA     | 2.18                     | 0.43              |
| 21:H:74:ALA:HB3   | 21:H:83:LEU:HD23   | 1.99                     | 0.43              |
| 21:H:123:GLU:HA   | 21:H:128:ARG:HA    | 2.00                     | 0.43              |
| 25:L:9:MET:HE3    | 25:L:86:ARG:N      | 2.33                     | 0.43              |
| 26:M:78:ARG:HG3   | 26:M:80:VAL:HG13   | 1.99                     | 0.43              |
| 27:N:26:THR:HG1   | 27:N:58:GLU:CG     | 2.32                     | 0.43              |
| 34:U:5:ARG:HA     | 34:U:71:VAL:HG21   | 2.01                     | 0.43              |
| 34:U:9:HIS:O      | 34:U:16:PHE:HB3    | 2.18                     | 0.43              |
| 35:V:31:HIS:NE2   | 35:V:34:TYR:HD2    | 2.15                     | 0.43              |
| 40:a:150:U:C2     | 40:a:151:C:C5      | 3.06                     | 0.43              |
| 40:a:197:A:N6     | 40:a:2430:A:H2'    | 2.34                     | 0.43              |
| 40:a:271:G:C2     | 40:a:272:A:C5      | 3.07                     | 0.43              |
| 40:a:577:G:OP1    | 40:a:2502:G:O2'    | 2.36                     | 0.43              |
| 40:a:838:C:C2     | 40:a:839:U:C6      | 3.07                     | 0.43              |
| 40:a:1141:U:H4'   | 40:a:1142:A:O4'    | 2.18                     | 0.43              |
| 40:a:2092:U:C2    | 40:a:2225:A:O2'    | 2.71                     | 0.43              |
| 40:a:2313:C:O3'   | 53:n:88:LYS:NZ     | 2.48                     | 0.43              |
| 53:n:132:VAL:CG2  | 53:n:152:LEU:CD2   | 2.97                     | 0.43              |
| 57:r:54:LEU:HA    | 57:r:57:LYS:HZ3    | 1.83                     | 0.43              |
| 62:w:96:ARG:O     | 62:w:113:ILE:HA    | 2.19                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 65:z:79:PHE:CE1   | 65:z:110:VAL:HA    | 2.46                     | 0.43              |
| 1:0:1:MET:HE3     | 1:0:43:ASN:OD1     | 2.18                     | 0.43              |
| 8:7:1:A:C6        | 10:B:37:A:N1       | 2.86                     | 0.43              |
| 9:9:118:ILE:HB    | 9:9:119:PRO:CD     | 2.42                     | 0.43              |
| 11:AA:557:ARG:HB3 | 11:AA:587:LEU:HD13 | 2.00                     | 0.43              |
| 12:AB:6:LEU:HD22  | 14:AE:291:ILE:HD11 | 1.99                     | 0.43              |
| 14:AE:1022:PRO:O  | 14:AE:1126:GLN:NE2 | 2.45                     | 0.43              |
| 14:AE:1321:SER:OG | 14:AE:1349:GLU:OE2 | 2.32                     | 0.43              |
| 10:B:19:G:N3      | 10:B:57:A:C4       | 2.87                     | 0.43              |
| 16:C:27:ALA:CA    | 16:C:30:LYS:HE3    | 2.49                     | 0.43              |
| 17:D:13:U:N3      | 17:D:915:A:C6      | 2.87                     | 0.43              |
| 17:D:76:G:C5      | 17:D:77:A:C8       | 3.06                     | 0.43              |
| 17:D:671:G:H4'    | 25:L:79:ARG:HH12   | 1.83                     | 0.43              |
| 18:E:22:ALA:CA    | 18:E:25:ARG:HE     | 2.31                     | 0.43              |
| 20:G:117:LEU:HD21 | 20:G:141:LEU:CA    | 2.48                     | 0.43              |
| 21:H:163:ARG:N    | 21:H:298:GLU:CG    | 2.81                     | 0.43              |
| 21:H:310:ASP:HB2  | 21:H:316:ILE:HD11  | 2.00                     | 0.43              |
| 21:H:332:VAL:CG1  | 21:H:335:ILE:HG13  | 2.47                     | 0.43              |
| 24:K:15:LEU:HD23  | 24:K:15:LEU:H      | 1.83                     | 0.43              |
| 25:L:25:TYR:O     | 25:L:26:THR:C      | 2.61                     | 0.43              |
| 32:S:86:GLU:O     | 32:S:90:ARG:HG2    | 2.17                     | 0.43              |
| 34:U:8:ARG:HD3    | 34:U:17:TYR:CE1    | 2.54                     | 0.43              |
| 40:a:39:G:H2'     | 40:a:40:U:H6       | 1.83                     | 0.43              |
| 40:a:68:G:N2      | 40:a:74:A:OP2      | 2.51                     | 0.43              |
| 40:a:533:G:H2'    | 40:a:534:U:C6      | 2.54                     | 0.43              |
| 40:a:870:U:N3     | 40:a:871:U:C5      | 2.86                     | 0.43              |
| 40:a:997:G:H5''   | 65:z:92:ARG:NH1    | 2.34                     | 0.43              |
| 40:a:1269:A:H2'   | 40:a:1270:C:C6     | 2.54                     | 0.43              |
| 40:a:1319:C:O2'   | 40:a:1320:C:H5'    | 2.18                     | 0.43              |
| 40:a:1443:U:H2'   | 40:a:1444:G:H8     | 1.82                     | 0.43              |
| 40:a:1665:A:O3'   | 59:t:66:LYS:CD     | 2.67                     | 0.43              |
| 40:a:1683:U:H2'   | 40:a:1684:G:H8     | 1.83                     | 0.43              |
| 40:a:2332:C:OP1   | 41:b:77:ARG:NH2    | 2.52                     | 0.43              |
| 43:d:46:A:C5      | 43:d:47:C:C5       | 3.06                     | 0.43              |
| 44:e:56:LEU:C     | 44:e:59:GLU:HG3    | 2.44                     | 0.43              |
| 46:g:59:ARG:HH11  | 46:g:63:ARG:CD     | 2.31                     | 0.43              |
| 47:h:45:ASN:OD1   | 47:h:46:ASN:N      | 2.51                     | 0.43              |
| 51:l:131:THR:HG22 | 51:l:160:ALA:O     | 2.18                     | 0.43              |
| 53:n:66:LEU:HD23  | 53:n:67:ILE:N      | 2.34                     | 0.43              |
| 53:n:79:ILE:O     | 53:n:79:ILE:HG13   | 2.18                     | 0.43              |
| 64:y:55:LEU:HA    | 64:y:77:HIS:CD2    | 2.54                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:0:46:GLU:HG2     | 1:0:48:LYS:NZ      | 2.32                     | 0.43              |
| 2:1:99:ARG:CZ      | 2:1:99:ARG:HB2     | 2.49                     | 0.43              |
| 3:2:37:ASP:OD2     | 3:2:37:ASP:C       | 2.62                     | 0.43              |
| 8:7:13:U:H3        | 23:J:47:ARG:NH1    | 2.10                     | 0.43              |
| 11:AA:813:GLU:HB2  | 14:AE:461:PHE:HD2  | 1.83                     | 0.43              |
| 11:AA:829:THR:HG23 | 11:AA:1059:ARG:HG2 | 1.99                     | 0.43              |
| 12:AB:2:GLN:HA     | 12:AB:59:PHE:C     | 2.43                     | 0.43              |
| 12:AB:109:THR:HA   | 12:AB:110:PRO:HD3  | 1.82                     | 0.43              |
| 14:AE:708:ASN:HA   | 14:AE:713:GLU:HA   | 2.00                     | 0.43              |
| 15:AF:58:LEU:HD12  | 15:AF:59:ILE:HG12  | 2.00                     | 0.43              |
| 17:D:416:G:C4      | 17:D:417:G:C8      | 3.07                     | 0.43              |
| 17:D:674:G:H2'     | 17:D:675:A:H8      | 1.84                     | 0.43              |
| 17:D:1149:C:N3     | 17:D:1150:A:N7     | 2.67                     | 0.43              |
| 17:D:1184:G:C2     | 17:D:1185:G:C8     | 3.07                     | 0.43              |
| 17:D:1194:U:H2'    | 17:D:1195:C:C6     | 2.54                     | 0.43              |
| 17:D:1408:A:H2'    | 17:D:1409:C:H6     | 1.84                     | 0.43              |
| 17:D:1477:U:H2'    | 17:D:1478:U:C6     | 2.53                     | 0.43              |
| 18:E:16:LYS:HA     | 18:E:19:LYS:HE3    | 2.00                     | 0.43              |
| 18:E:60:ARG:HG3    | 18:E:64:LYS:NZ     | 2.34                     | 0.43              |
| 20:G:23:TRP:CZ3    | 20:G:25:PRO:CA     | 3.01                     | 0.43              |
| 21:H:76:GLU:OE2    | 21:H:78:GLY:C      | 2.61                     | 0.43              |
| 21:H:303:LEU:CD2   | 21:H:305:HIS:HB3   | 2.48                     | 0.43              |
| 22:I:22:TRP:CZ2    | 22:I:32:ASN:CB     | 3.01                     | 0.43              |
| 22:I:69:HIS:CD2    | 22:I:104:ALA:HB3   | 2.54                     | 0.43              |
| 25:L:1:MET:HE2     | 25:L:67:PRO:N      | 2.34                     | 0.43              |
| 27:N:10:MET:HB2    | 27:N:33:LYS:HZ2    | 1.84                     | 0.43              |
| 27:N:66:PHE:C      | 27:N:67:GLN:OE1    | 2.62                     | 0.43              |
| 30:Q:84:VAL:HG11   | 30:Q:97:ILE:HD13   | 2.00                     | 0.43              |
| 31:R:57:LEU:HD23   | 31:R:59:ASN:CG     | 2.43                     | 0.43              |
| 33:T:63:ARG:HD2    | 33:T:67:LEU:HD23   | 2.01                     | 0.43              |
| 34:U:7:ALA:HA      | 34:U:28:ARG:HD3    | 2.01                     | 0.43              |
| 40:a:531:C:C5      | 40:a:2035:G:C2     | 3.07                     | 0.43              |
| 40:a:538:A:H2'     | 40:a:539:G:O4'     | 2.18                     | 0.43              |
| 40:a:573:U:O2'     | 40:a:574:A:H3'     | 2.19                     | 0.43              |
| 40:a:1169:A:N3     | 40:a:1169:A:O4'    | 2.51                     | 0.43              |
| 40:a:2332:C:P      | 41:b:77:ARG:HH21   | 2.42                     | 0.43              |
| 40:a:2547:A:H5'    | 59:t:29:HIS:NE2    | 2.34                     | 0.43              |
| 43:d:31:C:C2       | 43:d:32:U:C5       | 3.06                     | 0.43              |
| 45:f:10:THR:CB     | 45:f:56:LYS:NZ     | 2.81                     | 0.43              |
| 47:h:71:LYS:HB2    | 47:h:96:TYR:CZ     | 2.54                     | 0.43              |
| 48:i:17:ARG:CB     | 48:i:20:ASP:OD1    | 2.67                     | 0.43              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 52:m:26:ASN:HA    | 52:m:29:GLN:HE21    | 1.83                     | 0.43              |
| 61:v:53:MET:O     | 61:v:57:VAL:HG12    | 2.18                     | 0.43              |
| 61:v:72:PRO:C     | 61:v:73:ILE:HD12    | 2.43                     | 0.43              |
| 61:v:111:GLU:HG2  | 61:v:112:LEU:N      | 2.33                     | 0.43              |
| 62:w:12:ARG:NH1   | 62:w:20:MET:HE1     | 2.33                     | 0.43              |
| 62:w:33:ILE:CD1   | 62:w:112:TYR:HD1    | 2.32                     | 0.43              |
| 64:y:106:LYS:CA   | 64:y:109:ARG:NH2    | 2.81                     | 0.43              |
| 65:z:12:ALA:O     | 65:z:16:LYS:HG2     | 2.19                     | 0.43              |
| 10:A:22:G:OP2     | 10:A:22:G:C8        | 2.72                     | 0.43              |
| 12:AB:144:ASN:HA  | 12:AB:149:GLU:CD    | 2.44                     | 0.43              |
| 13:AD:78:ILE:HA   | 13:AD:81:ILE:HG22   | 2.00                     | 0.43              |
| 14:AE:287:ALA:HB2 | 14:AE:292:VAL:HG11  | 1.85                     | 0.43              |
| 14:AE:1036:ARG:HE | 14:AE:1081:VAL:HG21 | 1.83                     | 0.43              |
| 17:D:34:C:H2'     | 17:D:35:G:H8        | 1.83                     | 0.43              |
| 17:D:246:A:C2     | 17:D:282:A:C4       | 3.06                     | 0.43              |
| 17:D:619:U:O4'    | 23:J:128:ARG:CZ     | 2.67                     | 0.43              |
| 17:D:679:C:N3     | 17:D:680:C:C5       | 2.87                     | 0.43              |
| 17:D:682:G:C2     | 17:D:683:G:C8       | 3.06                     | 0.43              |
| 17:D:723:U:C2     | 19:F:49:LYS:HE3     | 2.54                     | 0.43              |
| 17:D:771:G:H2'    | 17:D:772:U:C6       | 2.54                     | 0.43              |
| 17:D:1103:C:O2    | 20:G:106:THR:HG21   | 2.18                     | 0.43              |
| 20:G:208:ARG:NH1  | 20:G:211:THR:CG2    | 2.82                     | 0.43              |
| 22:I:22:TRP:CH2   | 22:I:32:ASN:HB2     | 2.53                     | 0.43              |
| 25:L:29:ILE:HD12  | 25:L:29:ILE:H       | 1.83                     | 0.43              |
| 26:M:4:ARG:HG2    | 26:M:5:ARG:NH2      | 2.32                     | 0.43              |
| 31:R:23:ALA:O     | 31:R:25:GLU:OE1     | 2.36                     | 0.43              |
| 37:X:22:ILE:HG23  | 37:X:66:GLU:CD      | 2.43                     | 0.43              |
| 38:Y:14:ALA:O     | 38:Y:15:GLY:C       | 2.61                     | 0.43              |
| 39:Z:2:ILE:CG2    | 39:Z:5:ASP:H        | 2.28                     | 0.43              |
| 40:a:39:G:H2'     | 40:a:40:U:C6        | 2.53                     | 0.43              |
| 40:a:1095:A:O2'   | 40:a:1096:A:O4'     | 2.36                     | 0.43              |
| 40:a:1141:U:O2    | 40:a:1142:A:N6      | 2.52                     | 0.43              |
| 40:a:1587:G:H2'   | 40:a:1588:G:C8      | 2.54                     | 0.43              |
| 40:a:1792:G:H5'   | 47:h:204:VAL:CG2    | 2.49                     | 0.43              |
| 40:a:1900:A:N1    | 40:a:1970:A:C6      | 2.87                     | 0.43              |
| 40:a:2466:C:C2    | 40:a:2467:C:C5      | 3.06                     | 0.43              |
| 43:d:89:U:O2'     | 43:d:90:C:P         | 2.77                     | 0.43              |
| 48:i:55:ILE:HD13  | 62:w:112:TYR:CE2    | 2.54                     | 0.43              |
| 53:n:40:VAL:HG13  | 53:n:42:GLU:CD      | 2.43                     | 0.43              |
| 54:o:13:ARG:HG2   | 60:u:62:PRO:O       | 2.18                     | 0.43              |
| 61:v:1:MET:SD     | 61:v:44:ARG:HA      | 2.59                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:5:10:DT:H73    | 11:AA:62:TYR:HB3  | 1.99                     | 0.43              |
| 9:9:105:LYS:O    | 9:9:106:PHE:HB3   | 2.18                     | 0.43              |
| 10:A:19:G:N2     | 40:a:2112:G:C1'   | 2.82                     | 0.43              |
| 10:A:19:G:N3     | 10:A:57:A:C4      | 2.87                     | 0.43              |
| 10:A:57:A:O5'    | 10:A:58:A:P       | 2.77                     | 0.43              |
| 14:AE:230:SER:OG | 14:AE:231:GLY:N   | 2.49                     | 0.43              |
| 17:D:43:C:P      | 34:U:12:LYS:HE3   | 2.59                     | 0.43              |
| 17:D:384:G:H2'   | 17:D:385:C:C6     | 2.54                     | 0.43              |
| 17:D:553:A:H2'   | 17:D:554:A:H8     | 1.84                     | 0.43              |
| 17:D:792:A:H1'   | 17:D:794:A:N7     | 2.34                     | 0.43              |
| 19:F:3:VAL:HG22  | 30:Q:111:THR:HG23 | 2.01                     | 0.43              |
| 20:G:131:LYS:O   | 20:G:135:LEU:HD13 | 2.19                     | 0.43              |
| 22:I:54:ARG:NH2  | 22:I:56:VAL:CG2   | 2.82                     | 0.43              |
| 29:P:56:HIS:C    | 29:P:57:VAL:HG23  | 2.44                     | 0.43              |
| 33:T:3:LEU:HD23  | 33:T:4:SER:N      | 2.33                     | 0.43              |
| 35:V:63:GLU:HB2  | 35:V:73:TRP:CZ2   | 2.54                     | 0.43              |
| 36:W:45:ILE:HA   | 36:W:62:VAL:HG12  | 2.01                     | 0.43              |
| 36:W:68:GLY:HA3  | 46:g:59:ARG:HH22  | 1.82                     | 0.43              |
| 37:X:79:ARG:NH1  | 46:g:56:ARG:NH1   | 2.66                     | 0.43              |
| 38:Y:9:LYS:CE    | 38:Y:55:PRO:HB3   | 2.43                     | 0.43              |
| 38:Y:32:VAL:HG13 | 38:Y:58:ILE:HG21  | 2.00                     | 0.43              |
| 40:a:192:C:C5    | 40:a:193:U:C6     | 3.07                     | 0.43              |
| 40:a:814:C:C2    | 40:a:815:C:C5     | 3.07                     | 0.43              |
| 40:a:841:G:C6    | 40:a:938:G:C6     | 3.06                     | 0.43              |
| 40:a:1074:G:C6   | 40:a:1075:C:N4    | 2.87                     | 0.43              |
| 40:a:1114:C:H2'  | 40:a:1115:G:C8    | 2.54                     | 0.43              |
| 40:a:1695:G:N7   | 47:h:14:ARG:NH2   | 2.66                     | 0.43              |
| 40:a:1879:C:H2'  | 40:a:1880:U:O4'   | 2.18                     | 0.43              |
| 40:a:1913:A:OP2  | 40:a:1913:A:H3'   | 2.18                     | 0.43              |
| 40:a:2557:G:H2'  | 40:a:2558:C:H6    | 1.84                     | 0.43              |
| 40:a:2579:C:O3'  | 49:j:137:SER:OG   | 2.32                     | 0.43              |
| 40:a:2615:U:C2   | 48:i:4:GLN:HA     | 2.53                     | 0.43              |
| 40:a:2821:A:C2   | 40:a:2822:G:C4    | 3.07                     | 0.43              |
| 49:j:156:PHE:CE2 | 58:s:81:ILE:HD13  | 2.54                     | 0.43              |
| 49:j:181:ASP:HB3 | 49:j:186:LEU:HB2  | 1.99                     | 0.43              |
| 53:n:20:PHE:HB3  | 53:n:22:TYR:CE1   | 2.54                     | 0.43              |
| 58:s:1:MET:SD    | 58:s:2:LYS:C      | 3.02                     | 0.43              |
| 58:s:88:THR:OG1  | 58:s:91:GLU:HG3   | 2.18                     | 0.43              |
| 59:t:59:LYS:NZ   | 59:t:92:GLU:CG    | 2.81                     | 0.43              |
| 59:t:108:ARG:HG2 | 59:t:116:ILE:HD13 | 2.01                     | 0.43              |
| 2:1:95:ARG:C     | 2:1:95:ARG:HD2    | 2.44                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:2:76:ARG:CZ     | 3:2:77:ARG:O       | 2.67                     | 0.43              |
| 9:9:88:HIS:CB     | 9:9:89:PRO:CD      | 2.81                     | 0.43              |
| 11:AA:22:LEU:HB3  | 11:AA:655:VAL:HG11 | 2.01                     | 0.43              |
| 14:AE:513:MET:HE1 | 14:AE:579:LEU:HD13 | 2.01                     | 0.43              |
| 16:C:20:GLU:OE1   | 16:C:21:ILE:O      | 2.36                     | 0.43              |
| 17:D:316:C:C2     | 17:D:317:U:C5      | 3.06                     | 0.43              |
| 17:D:690:G:H2'    | 17:D:691:G:C8      | 2.54                     | 0.43              |
| 17:D:796:C:N3     | 17:D:797:C:C5      | 2.87                     | 0.43              |
| 17:D:1125:U:N3    | 17:D:1127:G:C8     | 2.86                     | 0.43              |
| 17:D:1127:G:C6    | 17:D:1128:C:C5     | 3.07                     | 0.43              |
| 17:D:1157:A:C2    | 17:D:1181:G:C5     | 3.06                     | 0.43              |
| 18:E:60:ARG:O     | 18:E:64:LYS:HD3    | 2.19                     | 0.43              |
| 19:F:31:GLU:CD    | 19:F:34:ARG:NH2    | 2.77                     | 0.43              |
| 20:G:26:LYS:CE    | 20:G:193:PRO:HG2   | 2.49                     | 0.43              |
| 21:H:31:ILE:O     | 21:H:31:ILE:HG13   | 2.18                     | 0.43              |
| 21:H:336:ASP:HB2  | 21:H:341:ARG:H     | 1.84                     | 0.43              |
| 22:I:14:ILE:HB    | 22:I:178:LEU:HD21  | 2.01                     | 0.43              |
| 22:I:134:MET:HG3  | 22:I:151:VAL:HG21  | 2.00                     | 0.43              |
| 23:J:41:HIS:ND1   | 23:J:44:ARG:CZ     | 2.82                     | 0.43              |
| 23:J:105:MET:HE3  | 23:J:171:LEU:HD13  | 1.97                     | 0.43              |
| 24:K:68:ARG:O     | 24:K:69:ARG:NH1    | 2.52                     | 0.43              |
| 24:K:157:ARG:HG2  | 24:K:159:LYS:HD3   | 2.01                     | 0.43              |
| 26:M:16:PRO:HB3   | 28:O:46:MET:CG     | 2.47                     | 0.43              |
| 31:R:80:ILE:CG2   | 31:R:81:LEU:N      | 2.82                     | 0.43              |
| 37:X:101:ARG:C    | 37:X:103:LYS:H     | 2.26                     | 0.43              |
| 40:a:523:C:O2     | 40:a:554:U:O2'     | 2.37                     | 0.43              |
| 40:a:685:A:N1     | 40:a:787:C:H1'     | 2.33                     | 0.43              |
| 40:a:996:A:N6     | 40:a:1160:G:C6     | 2.87                     | 0.43              |
| 40:a:1009:A:N3    | 40:a:1153:C:O2'    | 2.48                     | 0.43              |
| 40:a:1144:A:C5    | 40:a:1145:C:C5     | 3.07                     | 0.43              |
| 40:a:1443:U:H2'   | 40:a:1444:G:C8     | 2.54                     | 0.43              |
| 40:a:1707:G:C5    | 40:a:1708:C:C5     | 3.07                     | 0.43              |
| 40:a:1770:G:C5    | 40:a:1983:G:C6     | 3.07                     | 0.43              |
| 40:a:1789:A:OP2   | 47:h:221:ARG:NH1   | 2.52                     | 0.43              |
| 40:a:2477:U:O2    | 56:q:4:ARG:NH2     | 2.51                     | 0.43              |
| 40:a:2590:A:H2'   | 40:a:2591:C:H6     | 1.83                     | 0.43              |
| 40:a:2723:C:C5'   | 62:w:1:MET:HE3     | 2.49                     | 0.43              |
| 42:c:76:GLU:CD    | 42:c:76:GLU:C      | 2.87                     | 0.43              |
| 43:d:82:U:O2      | 45:f:53:PHE:HZ     | 2.02                     | 0.43              |
| 47:h:130:LEU:CD2  | 47:h:192:LEU:HD21  | 2.48                     | 0.43              |
| 47:h:183:LYS:CE   | 47:h:265:LYS:O     | 2.67                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:n:104:ILE:HD11  | 53:n:174:ASP:O     | 2.19                     | 0.43              |
| 59:t:118:LEU:O     | 59:t:119:ALA:C     | 2.62                     | 0.43              |
| 3:2:9:LYS:O        | 3:2:12:ARG:NH2     | 2.52                     | 0.42              |
| 8:7:21:U:H3'       | 8:7:21:U:C6        | 2.52                     | 0.42              |
| 9:9:15:VAL:HG22    | 9:9:66:GLY:HA3     | 2.00                     | 0.42              |
| 9:9:24:SER:O       | 9:9:96:PHE:CE1     | 2.72                     | 0.42              |
| 9:9:94:ARG:N       | 9:9:94:ARG:HD3     | 2.34                     | 0.42              |
| 10:A:47:U:O2'      | 10:A:50:U:OP1      | 2.37                     | 0.42              |
| 11:AA:590:PRO:HB2  | 11:AA:655:VAL:HG21 | 2.01                     | 0.42              |
| 11:AA:646:SER:OG   | 11:AA:647:ARG:N    | 2.52                     | 0.42              |
| 11:AA:861:ALA:HB1  | 11:AA:882:ILE:HD13 | 2.01                     | 0.42              |
| 11:AA:1313:HIS:CD2 | 15:AF:31:GLN:HE22  | 2.37                     | 0.42              |
| 12:AB:81:PHE:CD1   | 14:AE:141:PHE:O    | 2.72                     | 0.42              |
| 10:B:49:G:O5'      | 10:B:49:G:H8       | 2.01                     | 0.42              |
| 17:D:119:A:C2      | 17:D:240:G:C8      | 3.07                     | 0.42              |
| 17:D:320:A:H2'     | 17:D:321:A:O4'     | 2.19                     | 0.42              |
| 17:D:414:A:C2      | 17:D:415:A:H1'     | 2.54                     | 0.42              |
| 17:D:684:U:H2'     | 17:D:685:G:O4'     | 2.19                     | 0.42              |
| 17:D:953:G:O6      | 37:X:103:LYS:HE3   | 2.18                     | 0.42              |
| 17:D:1104:G:H4'    | 20:G:113:ARG:HH22  | 1.83                     | 0.42              |
| 17:D:1152:A:OP1    | 29:P:72:ARG:NH1    | 2.43                     | 0.42              |
| 17:D:1464:U:C2     | 17:D:1465:A:C8     | 3.07                     | 0.42              |
| 17:D:1499:A:H2'    | 17:D:1500:A:H8     | 1.84                     | 0.42              |
| 19:F:5:LYS:HD3     | 30:Q:109:ASN:OD1   | 2.20                     | 0.42              |
| 24:K:77:ASN:O      | 24:K:80:THR:O      | 2.37                     | 0.42              |
| 26:M:17:LYS:NZ     | 26:M:18:PHE:CE1    | 2.78                     | 0.42              |
| 26:M:23:LEU:H      | 26:M:23:LEU:CD1    | 2.30                     | 0.42              |
| 39:Z:29:LYS:O      | 39:Z:30:PHE:HD2    | 2.02                     | 0.42              |
| 40:a:471:A:H2'     | 40:a:472:A:O4'     | 2.19                     | 0.42              |
| 40:a:635:C:OP1     | 60:u:126:ARG:CZ    | 2.67                     | 0.42              |
| 40:a:858:G:OP1     | 41:b:78:LYS:HE3    | 2.18                     | 0.42              |
| 40:a:1008:A:OP2    | 58:s:37:ARG:NH1    | 2.52                     | 0.42              |
| 40:a:1028:A:N6     | 40:a:1125:G:H2'    | 2.34                     | 0.42              |
| 40:a:1139:G:O3'    | 58:s:26:GLY:HA3    | 2.19                     | 0.42              |
| 40:a:1223:G:N1     | 40:a:1226:A:OP2    | 2.49                     | 0.42              |
| 40:a:1282:U:H2'    | 40:a:1283:G:O4'    | 2.18                     | 0.42              |
| 40:a:1839:G:O4'    | 40:a:1927:A:O4'    | 2.37                     | 0.42              |
| 40:a:2037:A:H2'    | 40:a:2038:G:C8     | 2.54                     | 0.42              |
| 40:a:2215:C:H2'    | 40:a:2216:G:C8     | 2.54                     | 0.42              |
| 40:a:2377:A:O2'    | 63:x:117:PHE:O     | 2.36                     | 0.42              |
| 40:a:2462:C:C2     | 40:a:2463:C:C5     | 3.07                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 40:a:2845:U:H5''    | 64:y:52:ASN:O       | 2.19                     | 0.42              |
| 43:d:39:A:C2        | 43:d:44:G:C2        | 3.07                     | 0.42              |
| 43:d:57:A:N7        | 53:n:26:MET:CE      | 2.82                     | 0.42              |
| 46:g:47:LYS:CE      | 53:n:115:ARG:HA     | 2.49                     | 0.42              |
| 53:n:12:VAL:HG13    | 53:n:172:ALA:CB     | 2.49                     | 0.42              |
| 53:n:15:LYS:C       | 53:n:19:GLU:OE1     | 2.62                     | 0.42              |
| 58:s:125:TYR:CD2    | 58:s:130:HIS:HB3    | 2.54                     | 0.42              |
| 59:t:110:GLU:OE1    | 59:t:110:GLU:HA     | 2.19                     | 0.42              |
| 62:w:58:ASP:HB2     | 62:w:80:PHE:CE1     | 2.54                     | 0.42              |
| 63:x:14:ALA:O       | 63:x:15:ARG:C       | 2.61                     | 0.42              |
| 64:y:27:GLU:HB3     | 64:y:87:LYS:HZ1     | 1.83                     | 0.42              |
| 65:z:111:GLU:OE2    | 65:z:112:LYS:HD2    | 2.19                     | 0.42              |
| 4:3:35:ILE:HD11     | 4:3:62:GLU:C        | 2.44                     | 0.42              |
| 5:4:79:ARG:HA       | 5:4:79:ARG:HD3      | 1.82                     | 0.42              |
| 9:9:80:THR:O        | 40:a:1108:U:OP1     | 2.37                     | 0.42              |
| 9:9:118:ILE:CB      | 9:9:119:PRO:HD3     | 2.44                     | 0.42              |
| 9:9:129:LEU:N       | 9:9:130:PRO:CD      | 2.81                     | 0.42              |
| 11:AA:300:ASP:OD1   | 11:AA:313:ALA:N     | 2.51                     | 0.42              |
| 11:AA:699:LEU:HG    | 11:AA:799:ASN:HD22  | 1.85                     | 0.42              |
| 11:AA:1275:VAL:HG13 | 11:AA:1287:LEU:HD11 | 2.01                     | 0.42              |
| 12:AB:29:LEU:H      | 12:AB:56:PHE:HB2    | 1.84                     | 0.42              |
| 14:AE:859:PRO:HD2   | 14:AE:862:THR:HG21  | 2.00                     | 0.42              |
| 17:D:43:C:P         | 34:U:12:LYS:HZ2     | 2.42                     | 0.42              |
| 17:D:57:G:H2'       | 17:D:58:C:C6        | 2.54                     | 0.42              |
| 17:D:687:A:C2       | 17:D:704:A:C6       | 3.07                     | 0.42              |
| 17:D:689:C:H2'      | 17:D:690:G:O4'      | 2.18                     | 0.42              |
| 17:D:1060:U:OP1     | 32:S:85:ARG:NH1     | 2.48                     | 0.42              |
| 17:D:1125:U:O2'     | 17:D:1126:U:O5'     | 2.32                     | 0.42              |
| 17:D:1329:A:OP1     | 37:X:28:THR:CB      | 2.66                     | 0.42              |
| 17:D:1513:A:H2'     | 17:D:1514:G:H8      | 1.84                     | 0.42              |
| 21:H:124:LEU:O      | 21:H:127:ILE:O      | 2.36                     | 0.42              |
| 22:I:72:ARG:O       | 22:I:75:ILE:HG22    | 2.19                     | 0.42              |
| 23:J:139:PRO:N      | 23:J:182:PHE:CE2    | 2.88                     | 0.42              |
| 29:P:52:LEU:HB2     | 32:S:81:ARG:NH1     | 2.33                     | 0.42              |
| 31:R:3:THR:O        | 31:R:4:VAL:C        | 2.62                     | 0.42              |
| 32:S:77:PHE:HE1     | 32:S:93:ILE:CG2     | 2.30                     | 0.42              |
| 33:T:70:LEU:CD2     | 33:T:78:TYR:HA      | 2.49                     | 0.42              |
| 34:U:12:LYS:HD2     | 34:U:13:LYS:HG2     | 2.00                     | 0.42              |
| 34:U:14:ARG:CD      | 34:U:42:ILE:HG21    | 2.47                     | 0.42              |
| 36:W:17:LYS:O       | 36:W:21:LYS:HD3     | 2.19                     | 0.42              |
| 36:W:44:MET:HE1     | 36:W:62:VAL:HG22    | 2.01                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:W:69:HIS:ND1   | 36:W:74:PHE:HZ     | 2.17                     | 0.42              |
| 40:a:125:A:C6     | 52:m:10:LEU:HD13   | 2.54                     | 0.42              |
| 40:a:307:G:N1     | 40:a:310:A:OP2     | 2.47                     | 0.42              |
| 40:a:310:A:C2     | 40:a:330:A:C4      | 3.07                     | 0.42              |
| 40:a:607:U:N3     | 40:a:608:A:N7      | 2.66                     | 0.42              |
| 40:a:859:G:O2'    | 40:a:916:G:O6      | 2.37                     | 0.42              |
| 40:a:973:A:O4'    | 40:a:1188:U:C6     | 2.72                     | 0.42              |
| 40:a:1506:U:H2'   | 40:a:1507:C:C6     | 2.54                     | 0.42              |
| 40:a:2297:A:C2    | 40:a:2321:U:C5     | 3.07                     | 0.42              |
| 40:a:2465:C:O2    | 40:a:2465:C:H2'    | 2.18                     | 0.42              |
| 42:c:66:THR:O     | 42:c:69:ALA:N      | 2.53                     | 0.42              |
| 43:d:48:U:P       | 63:x:30:ARG:HH22   | 2.41                     | 0.42              |
| 44:e:20:ASN:O     | 44:e:24:GLU:HG2    | 2.20                     | 0.42              |
| 47:h:144:VAL:HG21 | 47:h:162:VAL:HG11  | 2.01                     | 0.42              |
| 49:j:151:THR:HG23 | 49:j:151:THR:O     | 2.19                     | 0.42              |
| 51:l:47:LYS:HA    | 51:l:51:GLU:CD     | 2.44                     | 0.42              |
| 53:n:93:GLY:O     | 53:n:94:GLU:C      | 2.61                     | 0.42              |
| 59:t:43:ILE:HD12  | 59:t:56:ASP:HB2    | 2.02                     | 0.42              |
| 64:y:106:LYS:CB   | 64:y:109:ARG:HH22  | 2.32                     | 0.42              |
| 65:z:76:TYR:CZ    | 65:z:80:ILE:HD11   | 2.54                     | 0.42              |
| 65:z:78:LYS:HG2   | 65:z:117:LEU:HD21  | 2.00                     | 0.42              |
| 6:5:10:DT:H2''    | 12:AB:71:ALA:H     | 1.79                     | 0.42              |
| 8:7:12:U:H4'      | 24:K:56:VAL:HG11   | 2.01                     | 0.42              |
| 11:AA:125:GLY:H   | 11:AA:495:ALA:HB1  | 1.84                     | 0.42              |
| 12:AB:146:ILE:CD1 | 29:P:88:MET:CG     | 2.87                     | 0.42              |
| 14:AE:362:ARG:H   | 14:AE:365:GLN:HE21 | 1.66                     | 0.42              |
| 10:B:57:A:O5'     | 10:B:58:A:P        | 2.77                     | 0.42              |
| 16:C:27:ALA:HB1   | 16:C:30:LYS:HE3    | 2.00                     | 0.42              |
| 16:C:34:THR:HB    | 16:C:38:LYS:N      | 2.34                     | 0.42              |
| 17:D:323:U:H2'    | 17:D:324:G:O4'     | 2.19                     | 0.42              |
| 17:D:563:A:C2     | 17:D:567:G:C6      | 3.07                     | 0.42              |
| 17:D:619:U:H1'    | 23:J:128:ARG:NH1   | 2.34                     | 0.42              |
| 17:D:1071:C:C5'   | 24:K:54:ARG:HH21   | 2.33                     | 0.42              |
| 21:H:309:MET:HE1  | 21:H:318:PRO:HG3   | 2.02                     | 0.42              |
| 23:J:76:TYR:HE1   | 23:J:86:THR:HG21   | 1.84                     | 0.42              |
| 25:L:2:ARG:C      | 25:L:65:GLU:OE1    | 2.62                     | 0.42              |
| 29:P:7:ARG:HA     | 29:P:75:ASP:OD1    | 2.20                     | 0.42              |
| 29:P:64:GLN:HG2   | 32:S:101:TRP:HH2   | 1.84                     | 0.42              |
| 30:Q:85:MET:HG3   | 30:Q:111:THR:HB    | 2.00                     | 0.42              |
| 32:S:63:ARG:HH22  | 32:S:70:PRO:HD3    | 1.85                     | 0.42              |
| 40:a:196:A:C5     | 40:a:805:G:C6      | 3.07                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:a:353:C:C2     | 40:a:354:A:C8      | 3.07                     | 0.42              |
| 40:a:553:G:C5     | 40:a:554:U:C5      | 3.07                     | 0.42              |
| 40:a:1064:C:H2'   | 40:a:1065:U:C6     | 2.55                     | 0.42              |
| 40:a:2249:U:H3'   | 40:a:2250:G:C5'    | 2.49                     | 0.42              |
| 40:a:2469:A:C6    | 40:a:2482:A:C8     | 3.08                     | 0.42              |
| 40:a:2615:U:H2'   | 40:a:2616:C:H6     | 1.83                     | 0.42              |
| 44:e:25:GLN:OE1   | 44:e:50:VAL:HG21   | 2.19                     | 0.42              |
| 49:j:152:PRO:HG3  | 49:j:156:PHE:CE1   | 2.53                     | 0.42              |
| 50:k:21:TYR:CE2   | 50:k:38:LYS:HB3    | 2.54                     | 0.42              |
| 50:k:34:LEU:HB3   | 50:k:51:GLU:OE2    | 2.19                     | 0.42              |
| 51:l:6:LYS:NZ     | 51:l:119:ILE:C     | 2.77                     | 0.42              |
| 51:l:105:LEU:O    | 51:l:109:LEU:HG    | 2.18                     | 0.42              |
| 53:n:38:MET:HE3   | 53:n:57:LEU:HD23   | 2.01                     | 0.42              |
| 53:n:92:ARG:CZ    | 53:n:92:ARG:HB3    | 2.47                     | 0.42              |
| 60:u:122:VAL:CG1  | 60:u:125:LEU:CD2   | 2.90                     | 0.42              |
| 61:v:31:PHE:C     | 61:v:104:GLU:OE1   | 2.62                     | 0.42              |
| 61:v:74:THR:HA    | 61:v:88:ASN:O      | 2.19                     | 0.42              |
| 62:w:38:LEU:HB3   | 62:w:39:PRO:HD3    | 2.02                     | 0.42              |
| 62:w:60:VAL:CG2   | 62:w:63:ARG:NH1    | 2.78                     | 0.42              |
| 64:y:106:LYS:HB3  | 64:y:109:ARG:HH22  | 1.84                     | 0.42              |
| 65:z:82:GLY:CA    | 65:z:117:LEU:HD11  | 2.48                     | 0.42              |
| 1:0:77:PHE:CD1    | 1:0:77:PHE:C       | 2.97                     | 0.42              |
| 2:1:36:LEU:CD2    | 2:1:48:LYS:HA      | 2.48                     | 0.42              |
| 3:2:42:GLU:OE1    | 3:2:42:GLU:HA      | 2.19                     | 0.42              |
| 4:3:7:ARG:O       | 4:3:25:VAL:O       | 2.36                     | 0.42              |
| 8:7:19:U:H5''     | 22:I:72:ARG:NH2    | 2.35                     | 0.42              |
| 10:A:11:A:H2'     | 10:A:12:G:C8       | 2.54                     | 0.42              |
| 11:AA:741:MET:HE3 | 11:AA:974:ARG:HH12 | 1.84                     | 0.42              |
| 12:AB:90:SER:HB2  | 12:AB:94:HIS:CE1   | 2.54                     | 0.42              |
| 12:AB:138:ARG:HD2 | 12:AB:154:VAL:C    | 2.44                     | 0.42              |
| 14:AE:71:LEU:HD12 | 14:AE:71:LEU:HA    | 1.78                     | 0.42              |
| 14:AE:907:HIS:ND1 | 14:AE:908:ILE:O    | 2.48                     | 0.42              |
| 10:B:18:G:H2'     | 10:B:57:A:C2       | 2.54                     | 0.42              |
| 16:C:44:ILE:CG2   | 21:H:340:ARG:HB2   | 2.49                     | 0.42              |
| 16:C:60:LYS:NZ    | 17:D:735:C:O5'     | 2.52                     | 0.42              |
| 17:D:283:U:C2     | 17:D:284:C:C6      | 3.06                     | 0.42              |
| 17:D:381:C:H2'    | 17:D:382:A:O4'     | 2.19                     | 0.42              |
| 17:D:662:U:H2'    | 17:D:663:A:C8      | 2.55                     | 0.42              |
| 17:D:768:A:C5     | 17:D:769:G:C8      | 3.08                     | 0.42              |
| 17:D:1107:C:OP1   | 22:I:172:ARG:HG3   | 2.19                     | 0.42              |
| 17:D:1152:A:P     | 29:P:72:ARG:HH22   | 2.43                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:D:1172:C:H2'   | 17:D:1173:U:H6    | 1.82                     | 0.42              |
| 17:D:1276:G:O5'   | 17:D:1276:G:H8    | 2.02                     | 0.42              |
| 17:D:1302:C:OP1   | 37:X:13:LYS:NZ    | 2.30                     | 0.42              |
| 17:D:1436:U:C2    | 17:D:1437:A:C8    | 3.07                     | 0.42              |
| 17:D:1437:A:C4    | 17:D:1438:G:C8    | 3.08                     | 0.42              |
| 18:E:9:LYS:CG     | 18:E:13:GLN:NE2   | 2.82                     | 0.42              |
| 18:E:50:ALA:O     | 18:E:54:MET:HG3   | 2.19                     | 0.42              |
| 19:F:14:VAL:O     | 19:F:18:ARG:HG3   | 2.19                     | 0.42              |
| 20:G:55:ALA:O     | 20:G:59:LYS:HG2   | 2.19                     | 0.42              |
| 20:G:134:ALA:HA   | 20:G:137:ARG:NE   | 2.35                     | 0.42              |
| 21:H:74:ALA:HB3   | 21:H:83:LEU:CD2   | 2.50                     | 0.42              |
| 22:I:36:ASP:OD1   | 22:I:57:ILE:HG21  | 2.19                     | 0.42              |
| 22:I:156:ARG:O    | 22:I:156:ARG:HG3  | 2.20                     | 0.42              |
| 22:I:183:ASP:HB3  | 22:I:204:LYS:HZ2  | 1.84                     | 0.42              |
| 23:J:117:LEU:HD23 | 23:J:154:ARG:HH21 | 1.84                     | 0.42              |
| 25:L:24:ARG:O     | 25:L:25:TYR:C     | 2.62                     | 0.42              |
| 28:O:51:PRO:HB3   | 28:O:103:PHE:HD2  | 1.83                     | 0.42              |
| 35:V:15:ASP:OD1   | 35:V:15:ASP:N     | 2.49                     | 0.42              |
| 37:X:3:ARG:CZ     | 53:n:110:ARG:HD2  | 2.49                     | 0.42              |
| 38:Y:14:ALA:C     | 38:Y:50:LYS:HD2   | 2.44                     | 0.42              |
| 38:Y:99:LYS:CE    | 38:Y:138:VAL:O    | 2.67                     | 0.42              |
| 40:a:367:G:C4     | 40:a:368:A:C8     | 3.07                     | 0.42              |
| 40:a:780:G:O2'    | 40:a:783:A:N6     | 2.53                     | 0.42              |
| 40:a:874:G:C6     | 40:a:904:G:C6     | 3.08                     | 0.42              |
| 40:a:938:G:C2     | 40:a:939:G:C8     | 3.08                     | 0.42              |
| 40:a:1076:C:H2'   | 40:a:1077:A:C8    | 2.54                     | 0.42              |
| 40:a:1275:A:N1    | 40:a:1295:C:O2'   | 2.50                     | 0.42              |
| 40:a:1361:G:H2'   | 40:a:1362:C:C6    | 2.55                     | 0.42              |
| 40:a:1565:C:OP1   | 47:h:18:LYS:HD2   | 2.19                     | 0.42              |
| 40:a:1709:U:H2'   | 40:a:1710:G:C8    | 2.55                     | 0.42              |
| 40:a:1906:G:C8    | 40:a:1929:G:C5    | 3.07                     | 0.42              |
| 40:a:2061:G:N3    | 40:a:2063:C:C5    | 2.87                     | 0.42              |
| 40:a:2093:G:P     | 57:r:22:LYS:CG    | 3.07                     | 0.42              |
| 40:a:2516:A:O2'   | 40:a:2517:C:H5'   | 2.18                     | 0.42              |
| 40:a:2554:U:H2'   | 40:a:2555:U:C6    | 2.55                     | 0.42              |
| 46:g:58:ASP:C     | 46:g:62:LYS:HZ1   | 2.28                     | 0.42              |
| 47:h:94:VAL:HG12  | 47:h:95:LEU:N     | 2.34                     | 0.42              |
| 49:j:68:PHE:CE1   | 49:j:79:LEU:HD21  | 2.54                     | 0.42              |
| 50:k:9:ILE:HG22   | 50:k:27:LYS:HZ1   | 1.84                     | 0.42              |
| 51:l:193:VAL:O    | 51:l:194:LYS:C    | 2.62                     | 0.42              |
| 53:n:73:SER:OG    | 53:n:80:ARG:HA    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 59:t:42:THR:HG23  | 59:t:44:LYS:HZ1   | 1.84                     | 0.42              |
| 63:x:83:LEU:HD23  | 63:x:88:LYS:HD3   | 2.02                     | 0.42              |
| 65:z:47:TYR:CZ    | 65:z:51:ARG:NH2   | 2.87                     | 0.42              |
| 3:2:26:LYS:CE     | 3:2:26:LYS:HA     | 2.50                     | 0.42              |
| 5:4:2:PHE:CD1     | 5:4:56:PHE:CE1    | 3.08                     | 0.42              |
| 8:7:7:U:H6        | 8:7:7:U:H3'       | 1.84                     | 0.42              |
| 10:A:18:G:H2'     | 10:A:57:A:C2      | 2.55                     | 0.42              |
| 14:AE:513:MET:HE2 | 14:AE:513:MET:HB3 | 1.79                     | 0.42              |
| 10:B:22:G:C8      | 10:B:22:G:OP2     | 2.72                     | 0.42              |
| 16:C:73:ARG:NH1   | 30:Q:113:VAL:CG1  | 2.76                     | 0.42              |
| 17:D:545:C:C5'    | 23:J:69:GLU:HG3   | 2.38                     | 0.42              |
| 17:D:946:A:C2     | 17:D:947:G:C5     | 3.08                     | 0.42              |
| 17:D:1410:A:H2'   | 17:D:1411:C:C6    | 2.54                     | 0.42              |
| 17:D:1439:G:H2'   | 17:D:1440:U:O4'   | 2.20                     | 0.42              |
| 17:D:1458:G:OP1   | 18:E:30:THR:OG1   | 2.30                     | 0.42              |
| 19:F:39:GLU:OE2   | 19:F:44:GLU:HA    | 2.18                     | 0.42              |
| 21:H:308:GLU:HB2  | 21:H:347:LYS:HB3  | 2.02                     | 0.42              |
| 22:I:72:ARG:HD3   | 22:I:75:ILE:H     | 1.84                     | 0.42              |
| 23:J:170:TRP:CD1  | 23:J:171:LEU:HG   | 2.54                     | 0.42              |
| 25:L:94:HIS:CG    | 25:L:95:ALA:N     | 2.88                     | 0.42              |
| 26:M:99:LEU:O     | 26:M:103:TRP:CG   | 2.73                     | 0.42              |
| 28:O:39:PHE:CD1   | 28:O:44:ALA:HB1   | 2.53                     | 0.42              |
| 28:O:80:ARG:O     | 28:O:84:THR:HG23  | 2.19                     | 0.42              |
| 30:Q:47:ALA:O     | 30:Q:52:PHE:HB2   | 2.19                     | 0.42              |
| 31:R:25:GLU:O     | 31:R:25:GLU:HG2   | 2.20                     | 0.42              |
| 31:R:66:TYR:CE2   | 31:R:68:GLY:HA2   | 2.55                     | 0.42              |
| 31:R:116:LYS:O    | 31:R:117:TYR:HD1  | 2.02                     | 0.42              |
| 33:T:71:LYS:NZ    | 33:T:78:TYR:CD2   | 2.87                     | 0.42              |
| 34:U:4:ILE:N      | 34:U:4:ILE:HD12   | 2.34                     | 0.42              |
| 37:X:71:ARG:CZ    | 46:g:50:ASP:O     | 2.67                     | 0.42              |
| 38:Y:81:LYS:N     | 38:Y:81:LYS:CD    | 2.79                     | 0.42              |
| 39:Z:14:MET:CG    | 39:Z:15:SER:H     | 2.26                     | 0.42              |
| 40:a:104:A:C4     | 40:a:105:C:C6     | 3.08                     | 0.42              |
| 40:a:136:G:H2'    | 40:a:137:U:C6     | 2.54                     | 0.42              |
| 40:a:580:U:C2     | 40:a:581:C:C5     | 3.07                     | 0.42              |
| 40:a:1824:G:H3'   | 47:h:52:ARG:HH12  | 1.84                     | 0.42              |
| 40:a:2049:G:H21   | 49:j:161:MET:HE2  | 1.84                     | 0.42              |
| 40:a:2585:U:O2    | 40:a:2585:U:O4'   | 2.37                     | 0.42              |
| 40:a:2759:G:O2'   | 55:p:35:ARG:NH1   | 2.52                     | 0.42              |
| 42:c:4:VAL:HG22   | 42:c:11:ARG:HG2   | 2.00                     | 0.42              |
| 53:n:33:LYS:CA    | 53:n:96:MET:SD    | 3.07                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:p:70:ALA:HA    | 55:p:73:ASN:HD22  | 1.84                     | 0.42              |
| 57:r:8:LYS:NZ     | 57:r:9:VAL:O      | 2.53                     | 0.42              |
| 57:r:114:GLU:OE2  | 57:r:133:GLN:N    | 2.53                     | 0.42              |
| 61:v:71:LYS:C     | 61:v:92:TRP:CE3   | 2.97                     | 0.42              |
| 3:2:6:ARG:HE      | 3:2:42:GLU:CD     | 2.27                     | 0.42              |
| 5:4:80:HIS:HE1    | 5:4:82:TYR:CG     | 2.37                     | 0.42              |
| 9:9:35:VAL:HG22   | 9:9:35:VAL:O      | 2.19                     | 0.42              |
| 10:A:8:U:O2'      | 10:A:47:U:O4      | 2.29                     | 0.42              |
| 12:AB:90:SER:HB2  | 12:AB:94:HIS:NE2  | 2.34                     | 0.42              |
| 16:C:30:LYS:HA    | 16:C:33:ILE:HG12  | 2.01                     | 0.42              |
| 17:D:197:A:N6     | 17:D:221:C:H4'    | 2.35                     | 0.42              |
| 17:D:552:U:H2'    | 17:D:553:A:H8     | 1.85                     | 0.42              |
| 17:D:1073:U:C2    | 17:D:1074:G:C8    | 3.07                     | 0.42              |
| 17:D:1315:U:H2'   | 17:D:1316:G:O4'   | 2.19                     | 0.42              |
| 17:D:1381:U:C4    | 17:D:1382:C:C5    | 3.07                     | 0.42              |
| 20:G:30:PHE:CG    | 20:G:45:LYS:NZ    | 2.87                     | 0.42              |
| 20:G:30:PHE:CE1   | 20:G:201:PRO:HG3  | 2.53                     | 0.42              |
| 21:H:135:LEU:CB   | 21:H:157:ILE:CB   | 2.97                     | 0.42              |
| 23:J:67:VAL:C     | 23:J:72:PHE:CE2   | 2.98                     | 0.42              |
| 23:J:153:SER:OG   | 23:J:156:LYS:NZ   | 2.53                     | 0.42              |
| 27:N:47:GLU:OE1   | 27:N:63:LEU:C     | 2.62                     | 0.42              |
| 28:O:35:LEU:CD2   | 28:O:45:ARG:HG2   | 2.49                     | 0.42              |
| 33:T:15:PHE:HD2   | 33:T:30:ALA:CB    | 2.31                     | 0.42              |
| 34:U:67:ILE:O     | 34:U:67:ILE:HG13  | 2.20                     | 0.42              |
| 37:X:71:ARG:NH1   | 46:g:51:VAL:O     | 2.52                     | 0.42              |
| 38:Y:99:LYS:HD2   | 38:Y:140:GLU:OE2  | 2.19                     | 0.42              |
| 40:a:587:C:O2     | 60:u:33:ARG:NH2   | 2.52                     | 0.42              |
| 40:a:1281:G:H2'   | 40:a:1282:U:C6    | 2.55                     | 0.42              |
| 40:a:2392:A:N3    | 60:u:55:MET:HE2   | 2.34                     | 0.42              |
| 40:a:2571:U:O2'   | 49:j:151:THR:HG23 | 2.20                     | 0.42              |
| 40:a:2708:G:O4'   | 62:w:71:ARG:NH1   | 2.52                     | 0.42              |
| 40:a:2756:U:N3    | 40:a:2758:A:C6    | 2.87                     | 0.42              |
| 40:a:2783:U:H2'   | 40:a:2784:U:H6    | 1.85                     | 0.42              |
| 40:a:2838:G:C6    | 40:a:2839:G:C5    | 3.08                     | 0.42              |
| 40:a:2856:A:C6    | 40:a:2862:G:C6    | 3.08                     | 0.42              |
| 40:a:2859:G:H2'   | 40:a:2860:A:C8    | 2.54                     | 0.42              |
| 49:j:61:THR:HG23  | 49:j:63:PRO:HD2   | 2.00                     | 0.42              |
| 53:n:4:LEU:HD11   | 53:n:101:GLU:CB   | 2.50                     | 0.42              |
| 55:p:94:TYR:HE1   | 55:p:152:ARG:HD2  | 1.83                     | 0.42              |
| 58:s:15:TRP:CE3   | 58:s:135:GLN:HB3  | 2.55                     | 0.42              |
| 59:t:116:ILE:HG13 | 59:t:117:SER:N    | 2.34                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 61:v:96:ILE:HA    | 61:v:100:LYS:HE3   | 2.00                     | 0.42              |
| 61:v:115:GLU:O    | 61:v:116:ALA:C     | 2.61                     | 0.42              |
| 64:y:110:ILE:O    | 64:y:110:ILE:HG13  | 2.19                     | 0.42              |
| 2:1:49:LYS:NZ     | 40:a:491:G:O6      | 2.50                     | 0.42              |
| 3:2:9:LYS:C       | 3:2:12:ARG:HH22    | 2.28                     | 0.42              |
| 3:2:57:VAL:HG22   | 3:2:58:VAL:N       | 2.35                     | 0.42              |
| 8:7:12:U:H3'      | 8:7:12:U:C6        | 2.53                     | 0.42              |
| 9:9:23:LEU:CA     | 9:9:118:ILE:HD11   | 2.50                     | 0.42              |
| 9:9:69:PHE:O      | 9:9:72:LEU:HD11    | 2.20                     | 0.42              |
| 9:9:87:GLU:OE1    | 9:9:91:ALA:O       | 2.38                     | 0.42              |
| 14:AE:74:LYS:HE2  | 14:AE:74:LYS:HB2   | 1.60                     | 0.42              |
| 14:AE:97:VAL:HG12 | 14:AE:101:ARG:HG3  | 2.02                     | 0.42              |
| 14:AE:412:LEU:HA  | 14:AE:415:VAL:HG22 | 2.01                     | 0.42              |
| 14:AE:609:TYR:HD2 | 14:AE:610:ARG:HD2  | 1.85                     | 0.42              |
| 14:AE:694:SER:OG  | 14:AE:738:ARG:NE   | 2.52                     | 0.42              |
| 17:D:5:U:O2       | 17:D:5:U:O4'       | 2.37                     | 0.42              |
| 17:D:21:G:H2'     | 17:D:22:G:C8       | 2.54                     | 0.42              |
| 17:D:299:G:H2'    | 17:D:300:A:C8      | 2.55                     | 0.42              |
| 17:D:393:A:C2     | 17:D:394:G:C8      | 3.07                     | 0.42              |
| 17:D:603:U:C2     | 17:D:604:G:C8      | 3.08                     | 0.42              |
| 17:D:611:C:O2     | 17:D:611:C:H2'     | 2.18                     | 0.42              |
| 17:D:673:A:H2'    | 17:D:674:G:H8      | 1.79                     | 0.42              |
| 17:D:980:C:H2'    | 17:D:981:U:H5'     | 2.01                     | 0.42              |
| 17:D:1499:A:O2'   | 17:D:1500:A:H5'    | 2.20                     | 0.42              |
| 19:F:5:LYS:CD     | 30:Q:109:ASN:OD1   | 2.68                     | 0.42              |
| 22:I:184:TYR:O    | 22:I:185:ASN:CG    | 2.63                     | 0.42              |
| 24:K:97:GLN:NE2   | 24:K:98:PRO:O      | 2.52                     | 0.42              |
| 24:K:111:MET:O    | 24:K:112:ARG:C     | 2.63                     | 0.42              |
| 24:K:123:VAL:O    | 24:K:124:LEU:HD23  | 2.20                     | 0.42              |
| 25:L:88:MET:SD    | 25:L:90:MET:HE3    | 2.60                     | 0.42              |
| 26:M:74:GLU:HG3   | 26:M:91:VAL:CG1    | 2.50                     | 0.42              |
| 28:O:116:VAL:HG11 | 29:P:62:ARG:HD3    | 2.02                     | 0.42              |
| 30:Q:20:VAL:CG1   | 30:Q:21:ALA:N      | 2.82                     | 0.42              |
| 37:X:25:VAL:O     | 37:X:25:VAL:HG13   | 2.19                     | 0.42              |
| 40:a:133:U:H2'    | 40:a:134:G:C8      | 2.54                     | 0.42              |
| 40:a:407:G:C2     | 40:a:408:G:C8      | 3.07                     | 0.42              |
| 40:a:667:U:H2'    | 40:a:668:A:O4'     | 2.20                     | 0.42              |
| 40:a:1065:U:O2'   | 40:a:1066:U:P      | 2.77                     | 0.42              |
| 40:a:1145:C:H2'   | 40:a:1146:C:H6     | 1.84                     | 0.42              |
| 40:a:1399:C:C2    | 40:a:1400:U:C5     | 3.08                     | 0.42              |
| 40:a:1597:A:H5''  | 40:a:1598:A:H5'    | 2.02                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:a:1874:C:H2'   | 40:a:1875:G:O4'    | 2.20                     | 0.42              |
| 40:a:2072:C:C2    | 40:a:2073:C:C5     | 3.08                     | 0.42              |
| 40:a:2287:A:N7    | 40:a:2289:G:C8     | 2.87                     | 0.42              |
| 40:a:2673:G:C2    | 40:a:2674:G:C8     | 3.08                     | 0.42              |
| 47:h:18:LYS:HE3   | 47:h:20:VAL:HG21   | 2.02                     | 0.42              |
| 49:j:91:THR:HG22  | 49:j:92:VAL:N      | 2.35                     | 0.42              |
| 49:j:170:VAL:HG13 | 49:j:194:PRO:CG    | 2.50                     | 0.42              |
| 51:l:170:ARG:NH1  | 51:l:175:ILE:HA    | 2.34                     | 0.42              |
| 60:u:123:ARG:C    | 60:u:125:LEU:HD22  | 2.45                     | 0.42              |
| 62:w:70:THR:O     | 62:w:71:ARG:HB2    | 2.20                     | 0.42              |
| 62:w:73:ASN:C     | 62:w:73:ASN:ND2    | 2.76                     | 0.42              |
| 63:x:36:TYR:CD2   | 63:x:37:ALA:N      | 2.88                     | 0.42              |
| 63:x:48:LEU:CD2   | 63:x:87:ILE:CD1    | 2.98                     | 0.42              |
| 2:1:74:ILE:HD12   | 2:1:74:ILE:N       | 2.34                     | 0.42              |
| 8:7:23:U:O2       | 8:7:23:U:H3'       | 2.19                     | 0.42              |
| 8:7:31:G:C2'      | 8:7:32:U:H5'       | 2.49                     | 0.42              |
| 9:9:129:LEU:HD12  | 9:9:130:PRO:CD     | 2.43                     | 0.42              |
| 10:A:59:A:C5      | 10:A:60:U:C5       | 3.08                     | 0.42              |
| 12:AB:5:TYR:HA    | 12:AB:88:VAL:CG2   | 2.49                     | 0.42              |
| 14:AE:79:LYS:HG3  | 14:AE:81:ARG:HH12  | 1.83                     | 0.42              |
| 14:AE:134:ASP:HB3 | 14:AE:159:ILE:HG21 | 2.02                     | 0.42              |
| 10:B:11:A:H2'     | 10:B:12:G:C8       | 2.54                     | 0.42              |
| 17:D:13:U:C2      | 17:D:914:A:C8      | 3.08                     | 0.42              |
| 17:D:68:G:H3'     | 17:D:69:G:H5''     | 2.01                     | 0.42              |
| 17:D:119:A:C4     | 17:D:240:G:N7      | 2.88                     | 0.42              |
| 17:D:374:A:C6     | 17:D:375:U:C4      | 3.08                     | 0.42              |
| 17:D:501:C:H1'    | 17:D:549:C:H1'     | 2.01                     | 0.42              |
| 17:D:505:G:C2     | 17:D:506:G:C5      | 3.07                     | 0.42              |
| 17:D:545:C:OP2    | 23:J:62:ARG:NH1    | 2.53                     | 0.42              |
| 17:D:611:C:N3     | 17:D:612:C:C5      | 2.87                     | 0.42              |
| 17:D:1172:C:C2    | 17:D:1173:U:C5     | 3.08                     | 0.42              |
| 17:D:1328:C:H5''  | 37:X:28:THR:HG21   | 2.01                     | 0.42              |
| 17:D:1381:U:N3    | 17:D:1382:C:C5     | 2.88                     | 0.42              |
| 17:D:1524:C:H2'   | 17:D:1525:G:C8     | 2.55                     | 0.42              |
| 22:I:105:GLU:CD   | 22:I:107:ARG:HH21  | 2.28                     | 0.42              |
| 22:I:172:ARG:NH1  | 22:I:174:PRO:HG3   | 2.35                     | 0.42              |
| 23:J:67:VAL:CG1   | 23:J:71:GLN:HB3    | 2.50                     | 0.42              |
| 24:K:123:VAL:C    | 24:K:124:LEU:HD23  | 2.45                     | 0.42              |
| 30:Q:85:MET:HB3   | 30:Q:113:VAL:HG21  | 2.00                     | 0.42              |
| 33:T:77:ARG:HA    | 33:T:77:ARG:NE     | 2.35                     | 0.42              |
| 34:U:26:ASN:ND2   | 34:U:31:ARG:CD     | 2.83                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:V:61:ILE:HA     | 35:V:75:LEU:HA     | 2.02                     | 0.42              |
| 36:W:66:MET:SD     | 36:W:66:MET:C      | 3.03                     | 0.42              |
| 38:Y:79:LEU:HD11   | 38:Y:132:ALA:HA    | 2.02                     | 0.42              |
| 40:a:136:G:H2'     | 40:a:137:U:H6      | 1.85                     | 0.42              |
| 40:a:209:C:N3      | 40:a:210:C:C5      | 2.87                     | 0.42              |
| 40:a:320:A:N3      | 51:l:163:ASN:ND2   | 2.67                     | 0.42              |
| 40:a:404:A:O2'     | 40:a:405:U:P       | 2.78                     | 0.42              |
| 40:a:579:G:H2'     | 40:a:580:U:H6      | 1.85                     | 0.42              |
| 40:a:639:U:H2'     | 40:a:640:C:H6      | 1.83                     | 0.42              |
| 40:a:729:G:C8      | 47:h:207:LYS:HD2   | 2.54                     | 0.42              |
| 40:a:751:A:C6      | 40:a:789:A:C5      | 3.08                     | 0.42              |
| 40:a:789:A:N1      | 52:m:3:ARG:NH2     | 2.68                     | 0.42              |
| 40:a:1170:C:O2     | 40:a:1170:C:H2'    | 2.18                     | 0.42              |
| 40:a:1509:A:N3     | 40:a:1510:G:C8     | 2.87                     | 0.42              |
| 40:a:1511:G:H2'    | 40:a:1512:C:H6     | 1.83                     | 0.42              |
| 40:a:1580:A:C8     | 40:a:1581:G:C8     | 3.08                     | 0.42              |
| 40:a:1657:U:H2'    | 40:a:1658:C:H6     | 1.83                     | 0.42              |
| 40:a:1827:U:O2'    | 40:a:1828:G:H5'    | 2.19                     | 0.42              |
| 40:a:2002:G:OP1    | 62:w:13:ASN:HA     | 2.20                     | 0.42              |
| 40:a:2066:C:O2'    | 40:a:2067:G:H5'    | 2.20                     | 0.42              |
| 40:a:2218:G:C5'    | 42:c:45:ARG:HH12   | 2.33                     | 0.42              |
| 40:a:2884:U:C2     | 48:i:40:ARG:CZ     | 3.02                     | 0.42              |
| 41:b:21:LEU:HD23   | 41:b:40:GLN:HA     | 2.00                     | 0.42              |
| 51:l:23:PHE:CD1    | 51:l:111:GLU:HG3   | 2.55                     | 0.42              |
| 53:n:30:ARG:C      | 53:n:158:THR:HG1   | 2.28                     | 0.42              |
| 55:p:109:PHE:CD1   | 55:p:152:ARG:NH1   | 2.88                     | 0.42              |
| 57:r:66:ASN:CG     | 57:r:135:HIS:HB2   | 2.44                     | 0.42              |
| 59:t:7:MET:C       | 59:t:18:ARG:NH1    | 2.77                     | 0.42              |
| 62:w:38:LEU:HD12   | 62:w:38:LEU:HA     | 1.72                     | 0.42              |
| 63:x:88:LYS:O      | 63:x:116:GLN:OE1   | 2.38                     | 0.42              |
| 63:x:88:LYS:HB3    | 63:x:116:GLN:OE1   | 2.20                     | 0.42              |
| 3:2:11:LEU:HD11    | 3:2:46:ALA:CB      | 2.50                     | 0.42              |
| 6:5:10:DT:C2       | 11:AA:62:TYR:HE2   | 2.37                     | 0.42              |
| 6:5:16:DG:N2       | 11:AA:445:ILE:HG21 | 2.34                     | 0.42              |
| 9:9:33:VAL:H       | 9:9:36:ASP:CG      | 2.28                     | 0.42              |
| 11:AA:998:LEU:HD21 | 11:AA:1015:ALA:HB2 | 2.02                     | 0.42              |
| 12:AB:145:LEU:C    | 12:AB:147:ASN:H    | 2.28                     | 0.42              |
| 10:B:5:G:C2'       | 10:B:6:G:C5'       | 2.98                     | 0.42              |
| 16:C:12:ARG:CB     | 21:H:264:GLU:CB    | 2.98                     | 0.42              |
| 16:C:33:ILE:O      | 21:H:338:GLU:HB3   | 2.19                     | 0.42              |
| 17:D:36:C:N4       | 17:D:37:U:C4       | 2.88                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:D:415:A:C4    | 17:D:416:G:C8     | 3.07                     | 0.42              |
| 17:D:539:A:H2'   | 17:D:540:G:C8     | 2.54                     | 0.42              |
| 17:D:745:G:H2'   | 17:D:746:A:H8     | 1.84                     | 0.42              |
| 17:D:1261:A:C5   | 17:D:1262:C:C6    | 3.07                     | 0.42              |
| 20:G:105:LYS:C   | 20:G:109:GLN:HE22 | 2.24                     | 0.42              |
| 21:H:86:ARG:O    | 21:H:89:ALA:HB3   | 2.20                     | 0.42              |
| 23:J:76:TYR:HE1  | 23:J:86:THR:CG2   | 2.33                     | 0.42              |
| 24:K:80:THR:OG1  | 24:K:81:LEU:N     | 2.53                     | 0.42              |
| 24:K:88:VAL:HG12 | 24:K:93:ARG:HG2   | 2.02                     | 0.42              |
| 26:M:23:LEU:N    | 26:M:23:LEU:CD1   | 2.81                     | 0.42              |
| 26:M:37:SER:HA   | 28:O:41:ARG:HH22  | 1.85                     | 0.42              |
| 29:P:59:LYS:HE2  | 29:P:62:ARG:CZ    | 2.50                     | 0.42              |
| 33:T:18:ASP:O    | 33:T:19:ALA:HB3   | 2.20                     | 0.42              |
| 38:Y:45:THR:HG21 | 38:Y:50:LYS:NZ    | 2.34                     | 0.42              |
| 40:a:700:G:H2'   | 40:a:701:G:O4'    | 2.20                     | 0.42              |
| 40:a:969:G:H2'   | 40:a:970:U:C6     | 2.54                     | 0.42              |
| 40:a:1080:A:C6   | 40:a:1081:U:C4    | 3.08                     | 0.42              |
| 40:a:1209:U:O2'  | 40:a:1237:A:N1    | 2.46                     | 0.42              |
| 40:a:1252:G:H1   | 65:z:37:GLN:HE21  | 1.68                     | 0.42              |
| 40:a:1560:G:C5   | 40:a:1561:C:C5    | 3.08                     | 0.42              |
| 40:a:2228:G:H2'  | 40:a:2229:U:C6    | 2.54                     | 0.42              |
| 40:a:2244:U:O2'  | 40:a:2245:U:H5'   | 2.20                     | 0.42              |
| 40:a:2291:U:H2'  | 40:a:2292:U:H6    | 1.85                     | 0.42              |
| 40:a:2756:U:C4   | 40:a:2759:G:O6    | 2.73                     | 0.42              |
| 43:d:83:G:O4'    | 45:f:53:PHE:CE2   | 2.72                     | 0.42              |
| 44:e:8:GLU:O     | 44:e:9:LYS:HD3    | 2.19                     | 0.42              |
| 47:h:71:LYS:CB   | 47:h:96:TYR:CZ    | 3.03                     | 0.42              |
| 49:j:37:VAL:HG13 | 49:j:48:ILE:CD1   | 2.49                     | 0.42              |
| 49:j:175:LEU:HB3 | 49:j:189:VAL:CG1  | 2.50                     | 0.42              |
| 51:l:77:ILE:O    | 51:l:77:ILE:HG22  | 2.19                     | 0.42              |
| 53:n:38:MET:HE3  | 53:n:57:LEU:CG    | 2.49                     | 0.42              |
| 54:o:22:PHE:CE1  | 54:o:62:LEU:HD23  | 2.55                     | 0.42              |
| 54:o:45:ARG:HB3  | 54:o:46:PRO:HD3   | 2.02                     | 0.42              |
| 59:t:7:MET:SD    | 59:t:18:ARG:HG3   | 2.59                     | 0.42              |
| 61:v:45:GLN:HE22 | 61:v:125:PRO:HD2  | 1.85                     | 0.42              |
| 61:v:49:ALA:O    | 61:v:50:ARG:C     | 2.62                     | 0.42              |
| 61:v:105:MET:HE1 | 61:v:113:ALA:HA   | 2.01                     | 0.42              |
| 2:1:23:LEU:CD2   | 2:1:39:THR:HG21   | 2.50                     | 0.42              |
| 2:1:75:PHE:HE2   | 2:1:77:ASP:OD2    | 2.02                     | 0.42              |
| 3:2:5:GLU:HA     | 44:e:22:LEU:HD21  | 2.02                     | 0.42              |
| 4:3:6:ARG:HG2    | 4:3:7:ARG:N       | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:9:11:ILE:O      | 9:9:15:VAL:HG23   | 2.20                     | 0.42              |
| 10:A:68:C:C4      | 10:A:69:C:C5      | 3.08                     | 0.42              |
| 12:AB:111:TYR:N   | 12:AB:114:ASP:OD2 | 2.51                     | 0.42              |
| 13:AD:76:GLU:HB3  | 13:AD:80:GLU:HB3  | 2.01                     | 0.42              |
| 16:C:60:LYS:CE    | 17:D:735:C:O4'    | 2.64                     | 0.42              |
| 17:D:105:G:C5     | 17:D:106:C:C4     | 3.08                     | 0.42              |
| 17:D:519:C:H2'    | 17:D:520:A:O4'    | 2.20                     | 0.42              |
| 17:D:520:A:C2'    | 31:R:70:GLU:OE1   | 2.67                     | 0.42              |
| 17:D:588:G:C4'    | 27:N:3:MET:HE1    | 2.48                     | 0.42              |
| 17:D:687:A:C8     | 17:D:701:U:C4     | 3.08                     | 0.42              |
| 17:D:820:U:H4'    | 17:D:821:G:OP2    | 2.20                     | 0.42              |
| 17:D:964:A:C2     | 17:D:969:A:N3     | 2.87                     | 0.42              |
| 17:D:1202:U:N3    | 32:S:82:ILE:HD13  | 2.35                     | 0.42              |
| 17:D:1217:C:P     | 32:S:9:ARG:HE     | 2.41                     | 0.42              |
| 17:D:1241:G:H2'   | 17:D:1242:G:H8    | 1.85                     | 0.42              |
| 19:F:39:GLU:OE1   | 19:F:44:GLU:OE1   | 2.38                     | 0.42              |
| 20:G:30:PHE:HA    | 20:G:45:LYS:NZ    | 2.35                     | 0.42              |
| 21:H:70:VAL:O     | 21:H:71:ALA:HB2   | 2.20                     | 0.42              |
| 22:I:6:HIS:CD2    | 32:S:89:MET:HB3   | 2.55                     | 0.42              |
| 22:I:132:ARG:CB   | 22:I:135:LYS:HE3  | 2.49                     | 0.42              |
| 29:P:88:MET:HE2   | 29:P:88:MET:HB2   | 1.89                     | 0.42              |
| 30:Q:35:THR:HA    | 30:Q:42:LEU:HG    | 2.01                     | 0.42              |
| 31:R:57:LEU:HG    | 31:R:58:THR:N     | 2.35                     | 0.42              |
| 36:W:40:ILE:HG22  | 36:W:67:VAL:HA    | 2.01                     | 0.42              |
| 38:Y:96:LYS:CD    | 38:Y:136:GLY:HA3  | 2.50                     | 0.42              |
| 38:Y:139:VAL:HG22 | 38:Y:140:GLU:H    | 1.82                     | 0.42              |
| 40:a:138:U:C5     | 40:a:142:A:C6     | 3.08                     | 0.42              |
| 40:a:299:A:C5     | 40:a:322:A:C2     | 3.07                     | 0.42              |
| 40:a:301:G:C4     | 40:a:302:C:C5     | 3.07                     | 0.42              |
| 40:a:1289:C:H2'   | 40:a:1290:C:H6    | 1.84                     | 0.42              |
| 40:a:1946:U:H2'   | 40:a:1947:C:H6    | 1.83                     | 0.42              |
| 40:a:2586:U:H2'   | 40:a:2587:A:O4'   | 2.20                     | 0.42              |
| 40:a:2636:C:O2'   | 49:j:45:TYR:CZ    | 2.70                     | 0.42              |
| 43:d:39:A:C2      | 43:d:44:G:C4      | 3.07                     | 0.42              |
| 44:e:13:GLU:O     | 44:e:14:LEU:C     | 2.63                     | 0.42              |
| 44:e:14:LEU:HA    | 44:e:17:GLU:OE1   | 2.20                     | 0.42              |
| 44:e:37:LEU:HD21  | 44:e:43:LEU:CD2   | 2.49                     | 0.42              |
| 47:h:108:LYS:CG   | 47:h:109:GLY:N    | 2.83                     | 0.42              |
| 49:j:57:ALA:O     | 49:j:60:VAL:HG12  | 2.19                     | 0.42              |
| 49:j:100:LEU:O    | 49:j:100:LEU:HD12 | 2.19                     | 0.42              |
| 52:m:4:THR:HG23   | 52:m:5:PHE:N      | 2.34                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 52:m:25:LYS:HG3  | 52:m:29:GLN:NE2   | 2.34                     | 0.42              |
| 52:m:25:LYS:O    | 52:m:28:ARG:N     | 2.52                     | 0.42              |
| 58:s:123:LYS:CD  | 58:s:132:HIS:HD2  | 2.33                     | 0.42              |
| 61:v:105:MET:HG2 | 61:v:117:PHE:CZ   | 2.55                     | 0.42              |
| 61:v:111:GLU:HA  | 61:v:114:ARG:NE   | 2.35                     | 0.42              |
| 62:w:18:GLN:HE22 | 62:w:22:ARG:NE    | 2.18                     | 0.42              |
| 63:x:79:ALA:CB   | 63:x:113:ALA:HB3  | 2.49                     | 0.42              |
| 1:0:40:MET:HE1   | 65:z:105:ALA:HB1  | 2.01                     | 0.41              |
| 1:0:52:PRO:HB3   | 65:z:89:GLU:CD    | 2.44                     | 0.41              |
| 12:AB:6:LEU:HB2  | 12:AB:56:PHE:CE1  | 2.54                     | 0.41              |
| 12:AB:31:PRO:HG2 | 12:AB:51:PHE:CD2  | 2.55                     | 0.41              |
| 14:AE:964:LYS:O  | 14:AE:976:THR:OG1 | 2.35                     | 0.41              |
| 10:B:59:A:C5     | 10:B:60:U:C5      | 3.08                     | 0.41              |
| 16:C:13:PHE:CG   | 16:C:51:TYR:CD1   | 3.08                     | 0.41              |
| 16:C:70:TYR:HE2  | 25:L:49:TYR:CZ    | 2.39                     | 0.41              |
| 17:D:255:G:H2'   | 17:D:256:U:C6     | 2.55                     | 0.41              |
| 17:D:1061:G:H5'  | 29:P:61:ALA:HB2   | 2.02                     | 0.41              |
| 17:D:1526:G:P    | 19:F:42:THR:HG23  | 2.59                     | 0.41              |
| 18:E:22:ALA:N    | 18:E:25:ARG:HE    | 2.17                     | 0.41              |
| 18:E:53:GLU:O    | 18:E:57:ILE:CD1   | 2.68                     | 0.41              |
| 20:G:56:GLU:HG2  | 20:G:198:PHE:CZ   | 2.55                     | 0.41              |
| 20:G:115:LYS:C   | 20:G:115:LYS:HD3  | 2.45                     | 0.41              |
| 21:H:54:LYS:HD3  | 21:H:58:GLY:HA2   | 2.02                     | 0.41              |
| 21:H:277:GLY:C   | 21:H:331:MET:HE3  | 2.45                     | 0.41              |
| 21:H:331:MET:SD  | 21:H:348:GLN:HG2  | 2.60                     | 0.41              |
| 22:I:155:GLY:HA2 | 22:I:163:ALA:HB1  | 2.02                     | 0.41              |
| 23:J:76:TYR:O    | 23:J:76:TYR:CD1   | 2.73                     | 0.41              |
| 29:P:45:ARG:CD   | 29:P:47:GLU:OE2   | 2.67                     | 0.41              |
| 30:Q:64:GLN:HB2  | 30:Q:99:ALA:HB2   | 2.01                     | 0.41              |
| 33:T:26:GLU:CG   | 33:T:27:VAL:N     | 2.83                     | 0.41              |
| 33:T:70:LEU:HG   | 33:T:78:TYR:HB2   | 2.02                     | 0.41              |
| 35:V:43:LYS:C    | 35:V:44:LEU:HD12  | 2.45                     | 0.41              |
| 35:V:48:ASP:HB3  | 35:V:75:LEU:CD2   | 2.49                     | 0.41              |
| 40:a:592:A:N3    | 54:o:4:ILE:HD11   | 2.35                     | 0.41              |
| 40:a:826:U:O2'   | 60:u:53:GLY:HA3   | 2.19                     | 0.41              |
| 40:a:1128:G:C6   | 40:a:2518:A:C6    | 3.08                     | 0.41              |
| 40:a:1172:C:C2'  | 40:a:1173:U:O4'   | 2.68                     | 0.41              |
| 40:a:1246:A:H2'  | 40:a:1247:A:O4'   | 2.20                     | 0.41              |
| 40:a:1542:U:H2'  | 40:a:1543:G:O4'   | 2.20                     | 0.41              |
| 40:a:1820:U:C2   | 47:h:201:MET:CE   | 3.03                     | 0.41              |
| 40:a:1906:G:C8   | 40:a:1929:G:C4    | 3.08                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:a:1964:G:H4'    | 40:a:1965:C:OP2   | 2.19                     | 0.41              |
| 40:a:2040:G:H2'    | 40:a:2041:U:O4'   | 2.20                     | 0.41              |
| 40:a:2226:C:H2'    | 40:a:2227:A:O4'   | 2.20                     | 0.41              |
| 40:a:2590:A:C2     | 40:a:2591:C:C5    | 3.08                     | 0.41              |
| 40:a:2627:G:O2'    | 40:a:2781:A:N1    | 2.43                     | 0.41              |
| 40:a:2722:G:C2'    | 40:a:2723:C:H5'   | 2.50                     | 0.41              |
| 40:a:2813:A:H2'    | 40:a:2814:A:H8    | 1.85                     | 0.41              |
| 47:h:196:GLY:O     | 47:h:198:ALA:N    | 2.53                     | 0.41              |
| 49:j:34:VAL:HG13   | 49:j:48:ILE:CG2   | 2.50                     | 0.41              |
| 50:k:9:ILE:HD12    | 50:k:51:GLU:HG2   | 2.01                     | 0.41              |
| 51:l:194:LYS:C     | 51:l:198:GLU:OE1  | 2.63                     | 0.41              |
| 53:n:67:ILE:CD1    | 53:n:87:CYS:HB3   | 2.50                     | 0.41              |
| 54:o:29:LEU:O      | 54:o:29:LEU:HG    | 2.19                     | 0.41              |
| 55:p:17:VAL:O      | 55:p:18:LYS:CE    | 2.65                     | 0.41              |
| 58:s:125:TYR:HE2   | 58:s:130:HIS:CB   | 2.32                     | 0.41              |
| 60:u:98:ALA:O      | 60:u:100:ILE:HG13 | 2.20                     | 0.41              |
| 61:v:104:GLU:CD    | 61:v:105:MET:H    | 2.28                     | 0.41              |
| 3:2:26:LYS:HA      | 3:2:26:LYS:HE3    | 2.02                     | 0.41              |
| 3:2:30:ILE:HG22    | 3:2:32:LEU:HD22   | 2.02                     | 0.41              |
| 4:3:6:ARG:N        | 4:3:9:ASP:OD2     | 2.49                     | 0.41              |
| 5:4:18:ARG:NH1     | 43:d:93:C:OP2     | 2.53                     | 0.41              |
| 11:AA:524:ILE:HD12 | 11:AA:712:SER:HB2 | 2.02                     | 0.41              |
| 11:AA:755:LYS:HD2  | 11:AA:755:LYS:HA  | 1.86                     | 0.41              |
| 17:D:112:G:N1      | 17:D:330:C:C5     | 2.89                     | 0.41              |
| 17:D:256:U:H2'     | 17:D:257:G:C8     | 2.55                     | 0.41              |
| 17:D:338:A:C5      | 17:D:339:C:C5     | 3.09                     | 0.41              |
| 17:D:429:U:H3      | 17:D:431:A:N6     | 2.18                     | 0.41              |
| 17:D:678:U:C2      | 17:D:679:C:C5     | 3.08                     | 0.41              |
| 17:D:860:A:H2'     | 17:D:861:G:O4'    | 2.20                     | 0.41              |
| 17:D:997:U:O2'     | 17:D:998:C:H5'    | 2.20                     | 0.41              |
| 17:D:1319:A:O2'    | 17:D:1323:G:N7    | 2.51                     | 0.41              |
| 22:I:66:VAL:HB     | 22:I:101:ILE:CD1  | 2.50                     | 0.41              |
| 22:I:149:ILE:HG13  | 22:I:202:ILE:HG12 | 2.01                     | 0.41              |
| 25:L:14:GLN:NE2    | 25:L:83:ALA:HB2   | 2.35                     | 0.41              |
| 26:M:93:PRO:O      | 26:M:96:ARG:HG2   | 2.21                     | 0.41              |
| 27:N:27:MET:CA     | 27:N:58:GLU:OE2   | 2.67                     | 0.41              |
| 28:O:97:GLU:HG2    | 28:O:98:LEU:N     | 2.35                     | 0.41              |
| 31:R:3:THR:O       | 31:R:6:GLN:HB2    | 2.20                     | 0.41              |
| 31:R:79:VAL:O      | 31:R:103:ASP:HB2  | 2.20                     | 0.41              |
| 32:S:10:GLU:OE1    | 32:S:63:ARG:HG3   | 2.21                     | 0.41              |
| 32:S:86:GLU:CD     | 32:S:90:ARG:HD3   | 2.45                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 40:a:1069:A:C2     | 40:a:1073:A:C8      | 3.08                     | 0.41              |
| 40:a:1588:G:N1     | 40:a:1589:U:O4      | 2.53                     | 0.41              |
| 40:a:1996:C:OP1    | 59:t:31:ARG:NE      | 2.52                     | 0.41              |
| 40:a:2310:C:O2'    | 53:n:74:VAL:HG12    | 2.20                     | 0.41              |
| 40:a:2547:A:H4'    | 59:t:29:HIS:NE2     | 2.34                     | 0.41              |
| 40:a:2650:U:C2     | 40:a:2651:C:C5      | 3.08                     | 0.41              |
| 43:d:57:A:C4       | 43:d:58:A:C8        | 3.07                     | 0.41              |
| 43:d:113:C:HO2'    | 63:x:46:GLU:CD      | 2.28                     | 0.41              |
| 44:e:2:LYS:HZ1     | 44:e:49:ASP:CA      | 2.33                     | 0.41              |
| 48:i:4:GLN:OE1     | 48:i:8:PRO:HD3      | 2.19                     | 0.41              |
| 49:j:5:VAL:HB      | 49:j:32:ASN:HD21    | 1.86                     | 0.41              |
| 51:l:46:GLN:O      | 51:l:88:ARG:NH2     | 2.53                     | 0.41              |
| 51:l:149:ILE:HG21  | 51:l:175:ILE:HD11   | 2.01                     | 0.41              |
| 53:n:136:ILE:HA    | 53:n:141:ILE:HG21   | 2.01                     | 0.41              |
| 57:r:8:LYS:HD2     | 57:r:13:GLY:O       | 2.20                     | 0.41              |
| 58:s:28:LEU:HD12   | 58:s:142:ILE:HG21   | 2.01                     | 0.41              |
| 62:w:45:ARG:O      | 62:w:49:GLU:CD      | 2.62                     | 0.41              |
| 3:2:3:ARG:HG3      | 3:2:5:GLU:OE1       | 2.20                     | 0.41              |
| 3:2:22:THR:O       | 3:2:25:GLU:HG2      | 2.20                     | 0.41              |
| 5:4:2:PHE:CZ       | 5:4:56:PHE:CZ       | 3.08                     | 0.41              |
| 5:4:77:VAL:HG21    | 5:4:79:ARG:HE       | 1.84                     | 0.41              |
| 6:5:10:DT:H2''     | 12:AB:69:ILE:CA     | 2.50                     | 0.41              |
| 8:7:26:A:H3'       | 14:AE:395:LYS:HZ3   | 1.85                     | 0.41              |
| 11:AA:469:VAL:HA   | 11:AA:472:GLU:HG2   | 2.01                     | 0.41              |
| 12:AB:152:HIS:HB3  | 12:AB:154:VAL:HG11  | 2.00                     | 0.41              |
| 14:AE:211:GLU:HA   | 14:AE:214:ARG:HD2   | 2.02                     | 0.41              |
| 14:AE:1272:SER:HB2 | 14:AE:1292:LEU:HD11 | 2.02                     | 0.41              |
| 16:C:40:VAL:HG13   | 21:H:339:ARG:CD     | 2.49                     | 0.41              |
| 17:D:21:G:N2       | 17:D:22:G:C6        | 2.88                     | 0.41              |
| 17:D:76:G:C5       | 17:D:77:A:N7        | 2.88                     | 0.41              |
| 17:D:250:A:O4'     | 17:D:252:U:C6       | 2.72                     | 0.41              |
| 17:D:1186:G:H4'    | 28:O:112:GLU:OE2    | 2.20                     | 0.41              |
| 17:D:1202:U:C2     | 32:S:82:ILE:HD13    | 2.55                     | 0.41              |
| 17:D:1288:A:H2'    | 17:D:1289:A:O4'     | 2.21                     | 0.41              |
| 17:D:1493:A:O2'    | 17:D:1494:G:P       | 2.78                     | 0.41              |
| 18:E:48:GLN:CD     | 18:E:49:LYS:N       | 2.78                     | 0.41              |
| 21:H:34:ASP:OD1    | 21:H:50:ALA:HB3     | 2.20                     | 0.41              |
| 21:H:309:MET:HE2   | 21:H:309:MET:HB3    | 1.93                     | 0.41              |
| 23:J:65:TYR:CE1    | 23:J:100:ASN:CG     | 2.98                     | 0.41              |
| 25:L:38:ARG:HA     | 25:L:38:ARG:HD3     | 1.93                     | 0.41              |
| 25:L:42:TRP:HB2    | 25:L:59:TYR:O       | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:M:18:PHE:CD2    | 26:M:59:LEU:HG     | 2.56                     | 0.41              |
| 33:T:64:ARG:CZ     | 33:T:89:ARG:HH12   | 2.33                     | 0.41              |
| 35:V:7:THR:C       | 35:V:8:LEU:HD12    | 2.46                     | 0.41              |
| 39:Z:29:LYS:C      | 39:Z:30:PHE:HD2    | 2.28                     | 0.41              |
| 40:a:126:A:OP1     | 52:m:45:SER:OG     | 2.37                     | 0.41              |
| 40:a:235:U:C2      | 40:a:236:C:C6      | 3.08                     | 0.41              |
| 40:a:271:G:C2      | 40:a:272:A:C4      | 3.08                     | 0.41              |
| 40:a:826:U:OP1     | 40:a:2428:G:H3'    | 2.20                     | 0.41              |
| 40:a:1958:C:O2'    | 40:a:1959:G:H5'    | 2.21                     | 0.41              |
| 40:a:2461:A:H2'    | 40:a:2462:C:C6     | 2.55                     | 0.41              |
| 40:a:2649:C:C2     | 40:a:2650:U:C6     | 3.09                     | 0.41              |
| 48:i:14:GLY:HA2    | 48:i:17:ARG:HG2    | 2.01                     | 0.41              |
| 53:n:38:MET:HE3    | 53:n:57:LEU:CD2    | 2.50                     | 0.41              |
| 55:p:52:PHE:CE1    | 55:p:69:ARG:HD3    | 2.55                     | 0.41              |
| 55:p:121:ILE:CD1   | 55:p:141:ILE:HG22  | 2.43                     | 0.41              |
| 59:t:113:MET:SD    | 59:t:113:MET:C     | 3.03                     | 0.41              |
| 61:v:95:LEU:C      | 61:v:96:ILE:HD13   | 2.45                     | 0.41              |
| 65:z:111:GLU:OE2   | 65:z:112:LYS:HG2   | 2.20                     | 0.41              |
| 9:9:2:ALA:HB3      | 9:9:6:GLN:HB2      | 2.01                     | 0.41              |
| 10:A:5:G:C2'       | 10:A:6:G:C5'       | 2.98                     | 0.41              |
| 11:AA:27:LEU:O     | 11:AA:528:ARG:NH1  | 2.43                     | 0.41              |
| 11:AA:310:ILE:HG21 | 11:AA:325:LEU:HB3  | 2.03                     | 0.41              |
| 11:AA:478:ARG:HD2  | 11:AA:492:MET:HA   | 2.02                     | 0.41              |
| 11:AA:1088:ASP:OD1 | 11:AA:1088:ASP:N   | 2.51                     | 0.41              |
| 12:AB:3:SER:HB3    | 12:AB:5:TYR:CE2    | 2.55                     | 0.41              |
| 12:AB:143:LEU:HD13 | 12:AB:150:ILE:HD11 | 2.02                     | 0.41              |
| 17:D:122:G:C4      | 17:D:123:U:C6      | 3.08                     | 0.41              |
| 17:D:124:C:H2'     | 17:D:125:U:H6      | 1.84                     | 0.41              |
| 17:D:407:U:C2      | 17:D:408:A:C8      | 3.08                     | 0.41              |
| 17:D:517:G:O2'     | 17:D:530:G:H4'     | 2.21                     | 0.41              |
| 17:D:1035:A:C6     | 17:D:1036:A:N7     | 2.88                     | 0.41              |
| 17:D:1073:U:O2     | 20:G:103:ASN:ND2   | 2.52                     | 0.41              |
| 17:D:1113:C:C2     | 17:D:1114:C:C5     | 3.08                     | 0.41              |
| 17:D:1189:U:H4'    | 22:I:10:ILE:CD1    | 2.50                     | 0.41              |
| 17:D:1255:G:O2'    | 17:D:1258:G:N3     | 2.48                     | 0.41              |
| 18:E:54:MET:HB2    | 18:E:54:MET:HE2    | 1.86                     | 0.41              |
| 20:G:101:LEU:HD22  | 20:G:157:LEU:HD11  | 1.99                     | 0.41              |
| 21:H:116:VAL:O     | 21:H:279:LYS:HG2   | 2.21                     | 0.41              |
| 21:H:287:LEU:HD23  | 21:H:318:PRO:HB2   | 2.02                     | 0.41              |
| 21:H:293:PHE:HA    | 21:H:302:GLY:O     | 2.20                     | 0.41              |
| 22:I:23:PHE:CD2    | 29:P:97:ASP:HB2    | 2.53                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:K:100:SER:O   | 24:K:103:THR:HG22 | 2.20                     | 0.41              |
| 27:N:96:MET:HE2  | 27:N:99:LEU:HD12  | 2.03                     | 0.41              |
| 29:P:40:ILE:HD12 | 29:P:73:LEU:HD22  | 2.02                     | 0.41              |
| 30:Q:20:VAL:HG12 | 30:Q:21:ALA:N     | 2.35                     | 0.41              |
| 31:R:21:VAL:HG23 | 31:R:21:VAL:O     | 2.19                     | 0.41              |
| 34:U:4:ILE:HG22  | 34:U:71:VAL:HG11  | 2.03                     | 0.41              |
| 38:Y:60:VAL:CG2  | 38:Y:66:PHE:CD1   | 3.03                     | 0.41              |
| 40:a:134:G:H2'   | 40:a:135:U:H6     | 1.85                     | 0.41              |
| 40:a:272:A:C2    | 40:a:273:G:C8     | 3.09                     | 0.41              |
| 40:a:320:A:H2'   | 51:l:131:THR:HG21 | 2.03                     | 0.41              |
| 40:a:888:C:C4    | 40:a:889:C:N4     | 2.88                     | 0.41              |
| 40:a:958:U:C4    | 61:v:40:ARG:NH1   | 2.88                     | 0.41              |
| 40:a:1427:A:H4'  | 40:a:1428:C:O4'   | 2.21                     | 0.41              |
| 40:a:1773:A:C8   | 40:a:1829:A:C8    | 3.08                     | 0.41              |
| 40:a:2097:A:H2'  | 40:a:2098:U:C6    | 2.55                     | 0.41              |
| 40:a:2526:G:O2'  | 56:q:1:MET:HG2    | 2.21                     | 0.41              |
| 40:a:2708:G:C2   | 40:a:2709:G:C8    | 3.08                     | 0.41              |
| 41:b:30:SER:HA   | 41:b:66:LYS:HD2   | 2.03                     | 0.41              |
| 42:c:3:ARG:CD    | 42:c:30:LEU:HD11  | 2.50                     | 0.41              |
| 47:h:53:HIS:NE2  | 47:h:219:THR:HG23 | 2.36                     | 0.41              |
| 47:h:91:ILE:HG21 | 47:h:103:TYR:HB3  | 2.03                     | 0.41              |
| 49:j:37:VAL:HG22 | 49:j:48:ILE:HD12  | 2.02                     | 0.41              |
| 49:j:55:LYS:HD3  | 49:j:55:LYS:C     | 2.45                     | 0.41              |
| 49:j:68:PHE:CZ   | 49:j:79:LEU:HD21  | 2.56                     | 0.41              |
| 50:k:26:ASN:OD1  | 50:k:28:ARG:CZ    | 2.69                     | 0.41              |
| 51:l:6:LYS:NZ    | 51:l:119:ILE:CG2  | 2.82                     | 0.41              |
| 51:l:170:ARG:CZ  | 51:l:174:GLY:O    | 2.66                     | 0.41              |
| 53:n:9:LYS:HE3   | 53:n:9:LYS:HB3    | 1.91                     | 0.41              |
| 53:n:16:LEU:HD11 | 53:n:169:LEU:HD12 | 2.03                     | 0.41              |
| 55:p:91:GLY:HA2  | 55:p:160:LYS:CD   | 2.50                     | 0.41              |
| 57:r:5:LEU:CD1   | 57:r:17:ASP:HB3   | 2.50                     | 0.41              |
| 62:w:28:LEU:HD23 | 62:w:48:VAL:HG21  | 2.03                     | 0.41              |
| 63:x:21:LEU:C    | 63:x:21:LEU:HD23  | 2.46                     | 0.41              |
| 3:2:19:LYS:HE2   | 3:2:84:TYR:OH     | 2.21                     | 0.41              |
| 6:5:23:DA:H2''   | 6:5:24:DC:C6      | 2.56                     | 0.41              |
| 8:7:1:A:H61      | 10:B:37:A:N6      | 2.19                     | 0.41              |
| 8:7:29:U:C3'     | 8:7:29:U:C6       | 3.04                     | 0.41              |
| 9:9:33:VAL:O     | 9:9:36:ASP:OD1    | 2.39                     | 0.41              |
| 9:9:77:VAL:O     | 9:9:77:VAL:CG1    | 2.66                     | 0.41              |
| 9:9:117:LEU:O    | 9:9:117:LEU:CD2   | 2.67                     | 0.41              |
| 10:A:19:G:O6     | 40:a:2112:G:P     | 2.79                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:A:31:G:H2'      | 10:A:32:C:C6       | 2.55                     | 0.41              |
| 11:AA:135:THR:HG22 | 11:AA:144:VAL:HG22 | 2.02                     | 0.41              |
| 11:AA:144:VAL:HG23 | 11:AA:515:MET:HB2  | 2.02                     | 0.41              |
| 11:AA:741:MET:SD   | 11:AA:974:ARG:NH2  | 2.93                     | 0.41              |
| 11:AA:849:GLU:HB2  | 11:AA:887:VAL:HG23 | 2.02                     | 0.41              |
| 12:AB:133:PRO:HA   | 12:AB:159:PHE:HE2  | 1.84                     | 0.41              |
| 13:AD:46:ILE:HD11  | 13:AD:224:LEU:HD13 | 2.02                     | 0.41              |
| 14:AE:282:LEU:HD23 | 14:AE:282:LEU:HA   | 1.92                     | 0.41              |
| 14:AE:975:ILE:HD11 | 14:AE:1003:LEU:HG  | 2.02                     | 0.41              |
| 17:D:124:C:H2'     | 17:D:125:U:C6      | 2.56                     | 0.41              |
| 17:D:306:A:C4      | 17:D:307:C:C6      | 3.08                     | 0.41              |
| 17:D:356:A:C5      | 17:D:357:G:C8      | 3.08                     | 0.41              |
| 17:D:376:G:O3'     | 34:U:5:ARG:NE      | 2.54                     | 0.41              |
| 17:D:671:G:O2'     | 25:L:79:ARG:NH1    | 2.54                     | 0.41              |
| 17:D:951:G:C6      | 17:D:1231:G:C6     | 3.08                     | 0.41              |
| 17:D:1174:G:H2'    | 17:D:1175:G:H5'    | 2.01                     | 0.41              |
| 17:D:1309:G:C8     | 37:X:98:ARG:NH2    | 2.88                     | 0.41              |
| 17:D:1382:C:O2     | 17:D:1382:C:H2'    | 2.19                     | 0.41              |
| 17:D:1411:C:H2'    | 17:D:1412:C:H6     | 1.85                     | 0.41              |
| 19:F:58:LYS:O      | 19:F:62:ARG:NE     | 2.45                     | 0.41              |
| 20:G:6:MET:HA      | 20:G:9:MET:SD      | 2.61                     | 0.41              |
| 21:H:322:VAL:HG12  | 21:H:323:ASN:HB2   | 2.02                     | 0.41              |
| 22:I:113:ALA:HB1   | 22:I:200:VAL:HG13  | 2.02                     | 0.41              |
| 25:L:9:MET:SD      | 25:L:57:ALA:HB1    | 2.60                     | 0.41              |
| 26:M:18:PHE:HD2    | 26:M:59:LEU:CD2    | 2.31                     | 0.41              |
| 27:N:83:LEU:HD11   | 31:R:4:VAL:CB      | 2.51                     | 0.41              |
| 28:O:50:GLN:OE1    | 28:O:50:GLN:HA     | 2.20                     | 0.41              |
| 29:P:79:PRO:HG2    | 29:P:102:LEU:HD11  | 2.03                     | 0.41              |
| 38:Y:34:ILE:HG22   | 38:Y:34:ILE:O      | 2.20                     | 0.41              |
| 40:a:16:C:O4'      | 48:i:15:MET:HE1    | 2.20                     | 0.41              |
| 40:a:62:U:O2       | 40:a:62:U:H2'      | 2.20                     | 0.41              |
| 40:a:235:U:H2'     | 40:a:236:C:H6      | 1.86                     | 0.41              |
| 40:a:458:G:N2      | 40:a:469:G:H2'     | 2.36                     | 0.41              |
| 40:a:920:A:H2'     | 40:a:921:C:H6      | 1.85                     | 0.41              |
| 40:a:1343:G:C8     | 40:a:1597:A:C6     | 3.08                     | 0.41              |
| 40:a:1651:G:P      | 62:w:40:LYS:NZ     | 2.94                     | 0.41              |
| 40:a:1778:U:C4     | 40:a:1784:A:C4     | 3.07                     | 0.41              |
| 40:a:2250:G:OP1    | 40:a:2275:C:O2'    | 2.25                     | 0.41              |
| 40:a:2259:U:C5     | 40:a:2427:C:N4     | 2.88                     | 0.41              |
| 40:a:2507:C:C2     | 40:a:2583:G:C2     | 3.07                     | 0.41              |
| 40:a:2511:U:C5'    | 49:j:130:GLN:OE1   | 2.69                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 40:a:2531:A:C4      | 40:a:2532:G:C8     | 3.09                     | 0.41              |
| 40:a:2884:U:P       | 48:i:40:ARG:NH2    | 2.93                     | 0.41              |
| 41:b:40:GLN:NE2     | 41:b:59:LEU:HD23   | 2.35                     | 0.41              |
| 51:l:31:VAL:HG21    | 51:l:104:ALA:CB    | 2.50                     | 0.41              |
| 51:l:170:ARG:HH22   | 51:l:176:ASP:H     | 1.68                     | 0.41              |
| 61:v:57:VAL:CG2     | 61:v:60:GLN:O      | 2.68                     | 0.41              |
| 62:w:98:LEU:CD1     | 62:w:114:GLU:OE2   | 2.68                     | 0.41              |
| 64:y:37:LYS:CA      | 64:y:37:LYS:HE3    | 2.49                     | 0.41              |
| 65:z:74:ILE:CD1     | 65:z:79:PHE:HA     | 2.40                     | 0.41              |
| 1:0:4:VAL:HG23      | 1:0:4:VAL:O        | 2.20                     | 0.41              |
| 1:0:74:ILE:HD13     | 1:0:87:GLN:OE1     | 2.20                     | 0.41              |
| 9:9:41:LEU:CD1      | 38:Y:117:THR:HG22  | 2.50                     | 0.41              |
| 10:A:9:G:O2'        | 10:A:45:G:H2'      | 2.20                     | 0.41              |
| 11:AA:805:MET:HE3   | 11:AA:805:MET:HB2  | 1.86                     | 0.41              |
| 12:AB:26:VAL:HG13   | 12:AB:58:GLU:H     | 1.84                     | 0.41              |
| 12:AB:132:GLU:HB3   | 12:AB:151:LYS:HE3  | 2.02                     | 0.41              |
| 12:AB:155:LYS:HB3   | 12:AB:158:GLU:CD   | 2.45                     | 0.41              |
| 14:AE:1003:LEU:HD23 | 14:AE:1018:ALA:HB2 | 2.02                     | 0.41              |
| 10:B:1:C:C5         | 10:B:2:G:N7        | 2.89                     | 0.41              |
| 17:D:643:C:C2       | 17:D:644:U:C5      | 3.08                     | 0.41              |
| 18:E:54:MET:CE      | 18:E:75:HIS:CE1    | 2.99                     | 0.41              |
| 19:F:66:ARG:NH2     | 19:F:67:ARG:HH22   | 2.19                     | 0.41              |
| 20:G:58:ASN:HB2     | 20:G:220:THR:OG1   | 2.21                     | 0.41              |
| 20:G:96:TRP:CH2     | 20:G:100:MET:CE    | 3.03                     | 0.41              |
| 21:H:309:MET:HE1    | 21:H:318:PRO:CA    | 2.51                     | 0.41              |
| 23:J:62:ARG:CG      | 23:J:72:PHE:CZ     | 3.02                     | 0.41              |
| 23:J:74:ASN:OD1     | 23:J:74:ASN:C      | 2.64                     | 0.41              |
| 25:L:1:MET:CE       | 25:L:67:PRO:HD3    | 2.50                     | 0.41              |
| 25:L:35:LYS:CG      | 25:L:36:ILE:N      | 2.84                     | 0.41              |
| 26:M:59:LEU:HA      | 26:M:59:LEU:HD23   | 1.93                     | 0.41              |
| 27:N:59:LEU:HD23    | 27:N:59:LEU:HA     | 1.93                     | 0.41              |
| 28:O:44:ALA:HA      | 28:O:47:VAL:HG22   | 2.03                     | 0.41              |
| 28:O:50:GLN:CA      | 28:O:53:GLU:OE1    | 2.69                     | 0.41              |
| 29:P:85:ASP:OD1     | 29:P:88:MET:CE     | 2.68                     | 0.41              |
| 32:S:10:GLU:CD      | 32:S:63:ARG:HD2    | 2.45                     | 0.41              |
| 36:W:17:LYS:HB3     | 36:W:21:LYS:NZ     | 2.36                     | 0.41              |
| 38:Y:100:ILE:HG13   | 38:Y:139:VAL:CB    | 2.51                     | 0.41              |
| 40:a:66:C:H42       | 40:a:74:A:N6       | 2.19                     | 0.41              |
| 40:a:67:U:C4        | 40:a:74:A:N6       | 2.89                     | 0.41              |
| 40:a:152:A:C6       | 40:a:153:U:C4      | 3.09                     | 0.41              |
| 40:a:319:G:H2'      | 40:a:320:A:O4'     | 2.20                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 40:a:340:A:H2'     | 40:a:341:C:O4'      | 2.19                     | 0.41              |
| 40:a:443:A:N1      | 51:l:40:ARG:NH2     | 2.68                     | 0.41              |
| 40:a:818:G:N1      | 40:a:1188:U:OP2     | 2.36                     | 0.41              |
| 40:a:985:C:O2      | 40:a:986:C:C6       | 2.73                     | 0.41              |
| 40:a:1829:A:C8     | 40:a:1830:C:C5      | 3.08                     | 0.41              |
| 40:a:1957:C:C2     | 40:a:1958:C:C5      | 3.09                     | 0.41              |
| 40:a:2024:G:C5     | 40:a:2040:G:C2      | 3.09                     | 0.41              |
| 40:a:2848:G:HO2'   | 40:a:2867:G:H22     | 1.60                     | 0.41              |
| 45:f:4:THR:O       | 45:f:5:ILE:HD13     | 2.20                     | 0.41              |
| 47:h:161:TYR:HB3   | 47:h:194:GLU:HG2    | 2.03                     | 0.41              |
| 47:h:165:VAL:HG12  | 47:h:175:ARG:NH2    | 2.35                     | 0.41              |
| 47:h:246:THR:N     | 47:h:250:VAL:O      | 2.49                     | 0.41              |
| 49:j:47:ALA:O      | 49:j:48:ILE:HD13    | 2.20                     | 0.41              |
| 50:k:21:TYR:CZ     | 50:k:38:LYS:CG      | 3.04                     | 0.41              |
| 51:l:194:LYS:O     | 51:l:195:GLN:C      | 2.64                     | 0.41              |
| 53:n:132:VAL:HG11  | 53:n:137:ILE:HD11   | 2.01                     | 0.41              |
| 55:p:149:ARG:HH12  | 55:p:154:PRO:HB3    | 1.85                     | 0.41              |
| 58:s:133:ALA:O     | 58:s:134:ALA:C      | 2.62                     | 0.41              |
| 62:w:46:ARG:HE     | 62:w:46:ARG:HB3     | 1.65                     | 0.41              |
| 62:w:60:VAL:HG22   | 62:w:63:ARG:HH11    | 1.80                     | 0.41              |
| 65:z:91:ASP:O      | 65:z:95:LEU:HG      | 2.20                     | 0.41              |
| 1:0:47:VAL:C       | 1:0:48:LYS:HD3      | 2.45                     | 0.41              |
| 2:1:31:GLN:H       | 2:1:31:GLN:CD       | 2.22                     | 0.41              |
| 5:4:48:MET:CE      | 5:4:85:LYS:HA       | 2.50                     | 0.41              |
| 6:5:27:DG:N2       | 7:6:3:DC:O2         | 2.53                     | 0.41              |
| 10:A:12:G:H2'      | 10:A:13:C:OP1       | 2.20                     | 0.41              |
| 11:AA:979:LEU:HD11 | 11:AA:1011:LEU:HD11 | 2.03                     | 0.41              |
| 12:AB:72:THR:HG22  | 12:AB:73:ARG:N      | 2.36                     | 0.41              |
| 12:AB:160:ARG:HG3  | 12:AB:161:LYS:H     | 1.85                     | 0.41              |
| 14:AE:247:PRO:HA   | 14:AE:250:ARG:HE    | 1.86                     | 0.41              |
| 14:AE:836:ARG:HG3  | 14:AE:869:CYS:HB3   | 2.02                     | 0.41              |
| 17:D:195:A:H5''    | 18:E:64:LYS:HZ1     | 1.85                     | 0.41              |
| 17:D:695:A:O5'     | 30:Q:53:ARG:CZ      | 2.69                     | 0.41              |
| 17:D:960:U:O2'     | 17:D:1223:C:H4'     | 2.20                     | 0.41              |
| 17:D:1251:A:H2'    | 17:D:1252:A:O4'     | 2.20                     | 0.41              |
| 17:D:1319:A:C8     | 17:D:1323:G:C5      | 3.08                     | 0.41              |
| 21:H:330:VAL:HB    | 21:H:344:LEU:HD23   | 2.01                     | 0.41              |
| 22:I:123:GLN:HB3   | 22:I:128:VAL:HG21   | 2.02                     | 0.41              |
| 24:K:45:ARG:CG     | 24:K:45:ARG:NE      | 2.72                     | 0.41              |
| 24:K:115:LEU:O     | 24:K:120:VAL:HG12   | 2.20                     | 0.41              |
| 28:O:50:GLN:HA     | 28:O:53:GLU:OE1     | 2.20                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:P:6:ILE:CG2     | 29:P:100:ILE:HG13 | 2.51                     | 0.41              |
| 33:T:70:LEU:HD23   | 33:T:78:TYR:HD1   | 1.85                     | 0.41              |
| 38:Y:23:VAL:HG23   | 38:Y:27:LEU:HD23  | 2.01                     | 0.41              |
| 40:a:370:G:C6      | 40:a:424:G:N7     | 2.89                     | 0.41              |
| 40:a:465:G:H2'     | 40:a:466:A:C8     | 2.56                     | 0.41              |
| 40:a:690:G:H2'     | 40:a:691:C:H6     | 1.85                     | 0.41              |
| 40:a:909:A:C4      | 40:a:912:C:C5     | 3.09                     | 0.41              |
| 40:a:967:U:H2'     | 40:a:968:C:C6     | 2.56                     | 0.41              |
| 40:a:1676:A:H2'    | 40:a:1677:A:C8    | 2.56                     | 0.41              |
| 40:a:1946:U:H2'    | 40:a:1947:C:C6    | 2.56                     | 0.41              |
| 40:a:2686:G:H2'    | 40:a:2687:U:C6    | 2.56                     | 0.41              |
| 43:d:113:C:O2'     | 63:x:46:GLU:CD    | 2.64                     | 0.41              |
| 47:h:189:ARG:HG3   | 47:h:190:ALA:N    | 2.36                     | 0.41              |
| 47:h:210:ALA:HA    | 47:h:213:TRP:CE3  | 2.56                     | 0.41              |
| 47:h:245:VAL:HA    | 47:h:250:VAL:O    | 2.20                     | 0.41              |
| 51:l:108:ILE:HD11  | 51:l:180:LEU:CD1  | 2.50                     | 0.41              |
| 52:m:26:ASN:HA     | 52:m:29:GLN:NE2   | 2.36                     | 0.41              |
| 53:n:66:LEU:HD23   | 53:n:67:ILE:C     | 2.45                     | 0.41              |
| 53:n:170:LEU:HB2   | 53:n:177:PHE:HZ   | 1.86                     | 0.41              |
| 55:p:89:LEU:HD22   | 55:p:162:VAL:HA   | 2.02                     | 0.41              |
| 58:s:1:MET:SD      | 58:s:2:LYS:O      | 2.79                     | 0.41              |
| 61:v:112:LEU:HD12  | 61:v:112:LEU:H    | 1.86                     | 0.41              |
| 61:v:112:LEU:CA    | 61:v:115:GLU:OE1  | 2.68                     | 0.41              |
| 62:w:18:GLN:CD     | 62:w:18:GLN:C     | 2.88                     | 0.41              |
| 62:w:78:LYS:HA     | 62:w:82:GLU:OE1   | 2.21                     | 0.41              |
| 63:x:15:ARG:C      | 63:x:19:GLN:NE2   | 2.78                     | 0.41              |
| 5:4:77:VAL:CG2     | 5:4:79:ARG:NE     | 2.78                     | 0.41              |
| 8:7:32:U:H4'       | 14:AE:322:ARG:NH1 | 2.35                     | 0.41              |
| 9:9:47:GLU:C       | 9:9:49:GLY:H      | 2.28                     | 0.41              |
| 9:9:94:ARG:O       | 9:9:98:GLU:HG2    | 2.21                     | 0.41              |
| 11:AA:616:ILE:HG13 | 11:AA:652:TYR:HB2 | 2.02                     | 0.41              |
| 12:AB:112:PRO:HA   | 12:AB:133:PRO:CG  | 2.49                     | 0.41              |
| 12:AB:148:LYS:HB3  | 12:AB:148:LYS:HE2 | 1.66                     | 0.41              |
| 14:AE:66:LYS:HB2   | 14:AE:69:GLU:HB2  | 2.02                     | 0.41              |
| 14:AE:367:GLY:HA3  | 14:AE:448:GLN:HB2 | 2.03                     | 0.41              |
| 16:C:44:ILE:HG22   | 21:H:340:ARG:HB2  | 2.02                     | 0.41              |
| 17:D:18:C:C2       | 17:D:19:A:C8      | 3.09                     | 0.41              |
| 17:D:120:A:O2'     | 17:D:122:G:N7     | 2.48                     | 0.41              |
| 17:D:695:A:OP1     | 30:Q:54:GLY:HA3   | 2.21                     | 0.41              |
| 17:D:908:A:H2'     | 17:D:909:A:H8     | 1.85                     | 0.41              |
| 17:D:963:G:C2      | 17:D:964:A:C8     | 3.09                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:D:1119:C:C2   | 17:D:1120:C:C5    | 3.09                     | 0.41              |
| 17:D:1368:A:OP1  | 28:O:116:VAL:HG23 | 2.20                     | 0.41              |
| 17:D:1515:G:H2'  | 17:D:1516:G:C8    | 2.54                     | 0.41              |
| 20:G:20:THR:O    | 20:G:23:TRP:CD1   | 2.74                     | 0.41              |
| 20:G:49:MET:HB3  | 20:G:49:MET:HE2   | 1.79                     | 0.41              |
| 20:G:117:LEU:CD2 | 20:G:141:LEU:HA   | 2.51                     | 0.41              |
| 22:I:147:LYS:CE  | 22:I:204:LYS:O    | 2.68                     | 0.41              |
| 23:J:197:GLU:HA  | 23:J:200:ILE:HD12 | 2.03                     | 0.41              |
| 26:M:47:LEU:HD21 | 26:M:58:GLU:HB3   | 2.03                     | 0.41              |
| 30:Q:49:GLY:C    | 30:Q:51:GLY:H     | 2.29                     | 0.41              |
| 30:Q:79:ILE:O    | 30:Q:105:PHE:CE1  | 2.72                     | 0.41              |
| 31:R:24:LEU:CD2  | 31:R:95:TYR:CE1   | 3.04                     | 0.41              |
| 31:R:25:GLU:CD   | 31:R:30:LYS:HE3   | 2.46                     | 0.41              |
| 34:U:25:ARG:HA   | 34:U:25:ARG:HD2   | 1.95                     | 0.41              |
| 34:U:34:GLU:OE1  | 34:U:60:TRP:NE1   | 2.54                     | 0.41              |
| 38:Y:57:VAL:CG2  | 38:Y:71:LYS:HD3   | 2.50                     | 0.41              |
| 38:Y:63:ASP:C    | 38:Y:65:SER:H     | 2.28                     | 0.41              |
| 38:Y:102:ARG:CZ  | 38:Y:139:VAL:HG21 | 2.50                     | 0.41              |
| 39:Z:6:GLN:CD    | 39:Z:10:ALA:HB2   | 2.45                     | 0.41              |
| 40:a:209:C:C2    | 40:a:210:C:C6     | 3.09                     | 0.41              |
| 40:a:749:A:H2'   | 40:a:749:A:N3     | 2.35                     | 0.41              |
| 40:a:975:A:H1'   | 40:a:990:A:C2     | 2.56                     | 0.41              |
| 40:a:1057:A:C2   | 40:a:1082:U:N3    | 2.89                     | 0.41              |
| 40:a:1558:C:O4'  | 40:a:1560:G:C8    | 2.74                     | 0.41              |
| 40:a:1945:G:H2'  | 40:a:1946:U:C6    | 2.56                     | 0.41              |
| 40:a:2205:A:H2'  | 40:a:2206:C:C6    | 2.56                     | 0.41              |
| 40:a:2639:A:H2'  | 40:a:2640:G:O4'   | 2.21                     | 0.41              |
| 43:d:57:A:N7     | 53:n:26:MET:HE3   | 2.36                     | 0.41              |
| 48:i:28:LEU:CB   | 48:i:37:LYS:HE3   | 2.51                     | 0.41              |
| 49:j:11:MET:HE3  | 49:j:11:MET:HB3   | 1.63                     | 0.41              |
| 49:j:146:ILE:HA  | 49:j:159:LYS:NZ   | 2.36                     | 0.41              |
| 49:j:175:LEU:HB3 | 49:j:189:VAL:HG12 | 2.02                     | 0.41              |
| 49:j:184:ARG:NH2 | 64:y:7:GLN:CD     | 2.72                     | 0.41              |
| 53:n:138:PHE:O   | 53:n:141:ILE:HG22 | 2.21                     | 0.41              |
| 57:r:54:LEU:HD12 | 57:r:57:LYS:HE2   | 2.03                     | 0.41              |
| 62:w:49:GLU:OE2  | 62:w:95:THR:CG2   | 2.69                     | 0.41              |
| 1:0:77:PHE:HE1   | 1:0:79:ARG:HA     | 1.85                     | 0.41              |
| 4:3:6:ARG:NH1    | 40:a:84:A:C2'     | 2.84                     | 0.41              |
| 4:3:84:GLY:C     | 4:3:95:PHE:CE2    | 2.99                     | 0.41              |
| 8:7:13:U:C6      | 8:7:13:U:C3'      | 3.03                     | 0.41              |
| 9:9:17:GLU:OE2   | 9:9:53:ARG:NH2    | 2.53                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:9:31:ARG:NH1    | 40:a:1054:A:C1'    | 2.80                     | 0.41              |
| 9:9:95:LEU:O      | 9:9:98:GLU:HG2     | 2.20                     | 0.41              |
| 9:9:139:LEU:HD22  | 39:Z:11:VAL:HG22   | 2.02                     | 0.41              |
| 11:AA:22:LEU:HD22 | 11:AA:603:ILE:HG21 | 2.02                     | 0.41              |
| 12:AB:36:GLU:O    | 12:AB:37:LYS:HD2   | 2.21                     | 0.41              |
| 13:AD:22:THR:OG1  | 13:AD:207:THR:OG1  | 2.36                     | 0.41              |
| 14:AE:210:SER:O   | 14:AE:214:ARG:N    | 2.43                     | 0.41              |
| 10:B:12:G:H2'     | 10:B:13:C:OP1      | 2.20                     | 0.41              |
| 10:B:31:G:H2'     | 10:B:32:C:C6       | 2.55                     | 0.41              |
| 10:B:38:A:H4'     | 17:D:790:A:C1'     | 2.49                     | 0.41              |
| 16:C:12:ARG:NH1   | 16:C:13:PHE:CD1    | 2.89                     | 0.41              |
| 16:C:44:ILE:HG21  | 21:H:339:ARG:C     | 2.45                     | 0.41              |
| 16:C:54:GLN:HG3   | 16:C:55:LEU:H      | 1.85                     | 0.41              |
| 17:D:71:A:C6      | 17:D:100:G:N7      | 2.89                     | 0.41              |
| 17:D:124:C:C2     | 17:D:125:U:C5      | 3.08                     | 0.41              |
| 17:D:338:A:H2'    | 17:D:339:C:H6      | 1.85                     | 0.41              |
| 17:D:375:U:H1'    | 34:U:28:ARG:NH2    | 2.36                     | 0.41              |
| 17:D:414:A:C2     | 17:D:415:A:N9      | 2.89                     | 0.41              |
| 17:D:437:U:H5''   | 23:J:152:GLN:CD    | 2.46                     | 0.41              |
| 17:D:602:A:H2'    | 17:D:603:U:H6      | 1.86                     | 0.41              |
| 17:D:718:A:C2     | 30:Q:118:HIS:CE1   | 3.09                     | 0.41              |
| 17:D:920:U:H2'    | 17:D:921:U:C6      | 2.56                     | 0.41              |
| 17:D:985:C:C2     | 17:D:986:U:C5      | 3.08                     | 0.41              |
| 17:D:986:U:H2'    | 17:D:987:G:O4'     | 2.19                     | 0.41              |
| 18:E:9:LYS:HG2    | 18:E:13:GLN:NE2    | 2.36                     | 0.41              |
| 20:G:85:LEU:HD23  | 20:G:85:LEU:C      | 2.46                     | 0.41              |
| 21:H:267:TRP:CD2  | 21:H:340:ARG:HG3   | 2.56                     | 0.41              |
| 21:H:308:GLU:HG2  | 21:H:309:MET:N     | 2.31                     | 0.41              |
| 22:I:8:ASN:O      | 22:I:12:LEU:CD2    | 2.69                     | 0.41              |
| 24:K:46:VAL:HG12  | 24:K:47:GLY:N      | 2.36                     | 0.41              |
| 26:M:108:ALA:O    | 26:M:119:ARG:NE    | 2.51                     | 0.41              |
| 27:N:83:LEU:HD21  | 31:R:4:VAL:HG21    | 2.02                     | 0.41              |
| 28:O:21:ILE:HD12  | 28:O:86:ALA:CB     | 2.50                     | 0.41              |
| 28:O:25:ASN:HB2   | 28:O:27:LYS:NZ     | 2.36                     | 0.41              |
| 29:P:22:THR:HG21  | 29:P:72:ARG:HG3    | 2.03                     | 0.41              |
| 30:Q:75:LYS:HG3   | 30:Q:76:GLU:N      | 2.35                     | 0.41              |
| 30:Q:76:GLU:OE1   | 30:Q:76:GLU:HA     | 2.21                     | 0.41              |
| 31:R:57:LEU:HD23  | 31:R:59:ASN:OD1    | 2.20                     | 0.41              |
| 32:S:91:GLY:C     | 32:S:92:GLU:OE1    | 2.62                     | 0.41              |
| 33:T:67:LEU:CD1   | 33:T:78:TYR:CE1    | 3.04                     | 0.41              |
| 34:U:19:VAL:HG11  | 34:U:52:LEU:CD2    | 2.50                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:U:73:ALA:HA   | 34:U:76:LYS:HE2   | 2.03                     | 0.41              |
| 35:V:31:HIS:HD2  | 35:V:34:TYR:HB2   | 1.85                     | 0.41              |
| 37:X:3:ARG:NH2   | 46:g:35:ASP:HB2   | 2.36                     | 0.41              |
| 37:X:71:ARG:NH1  | 37:X:72:GLU:CG    | 2.84                     | 0.41              |
| 38:Y:82:ALA:CB   | 38:Y:108:ILE:HD12 | 2.50                     | 0.41              |
| 40:a:151:C:C2    | 40:a:152:A:N7     | 2.89                     | 0.41              |
| 40:a:205:G:O2'   | 40:a:206:U:OP2    | 2.39                     | 0.41              |
| 40:a:239:C:O2'   | 40:a:622:G:O2'    | 2.32                     | 0.41              |
| 40:a:485:C:N3    | 40:a:486:C:C5     | 2.89                     | 0.41              |
| 40:a:529:A:C4    | 40:a:2023:C:C5    | 3.09                     | 0.41              |
| 40:a:814:C:N3    | 40:a:815:C:C5     | 2.89                     | 0.41              |
| 40:a:841:G:H2'   | 40:a:842:U:H6     | 1.86                     | 0.41              |
| 40:a:1026:G:C8   | 40:a:1134:A:C4    | 3.08                     | 0.41              |
| 40:a:1142:A:N3   | 40:a:1142:A:H2'   | 2.36                     | 0.41              |
| 40:a:1212:G:O2'  | 40:a:1236:G:N2    | 2.47                     | 0.41              |
| 40:a:1289:C:H2'  | 40:a:1290:C:C6    | 2.56                     | 0.41              |
| 40:a:1365:A:H4'  | 42:c:11:ARG:HH12  | 1.85                     | 0.41              |
| 40:a:1430:G:H2'  | 40:a:1431:A:C8    | 2.56                     | 0.41              |
| 40:a:1799:G:N7   | 47:h:178:SER:OG   | 2.45                     | 0.41              |
| 40:a:1843:C:H2'  | 40:a:1844:C:H6    | 1.85                     | 0.41              |
| 40:a:2065:C:N3   | 40:a:2066:C:C5    | 2.89                     | 0.41              |
| 40:a:2072:C:C2   | 40:a:2073:C:C6    | 3.08                     | 0.41              |
| 40:a:2366:A:H2'  | 40:a:2367:G:O4'   | 2.21                     | 0.41              |
| 40:a:2454:G:C5   | 40:a:2455:G:C8    | 3.09                     | 0.41              |
| 40:a:2569:G:C2   | 40:a:2570:G:C8    | 3.09                     | 0.41              |
| 40:a:2589:A:H2'  | 40:a:2590:A:H8    | 1.86                     | 0.41              |
| 40:a:2619:C:O2'  | 40:a:2620:C:H5'   | 2.21                     | 0.41              |
| 40:a:2784:U:H2'  | 40:a:2785:C:C6    | 2.55                     | 0.41              |
| 40:a:2808:G:N1   | 40:a:2891:U:C5    | 2.89                     | 0.41              |
| 40:a:2848:G:N2   | 40:a:2867:G:C4    | 2.89                     | 0.41              |
| 41:b:55:ARG:CZ   | 41:b:55:ARG:CA    | 2.99                     | 0.41              |
| 41:b:70:GLU:HG3  | 41:b:72:LYS:HG2   | 2.03                     | 0.41              |
| 42:c:67:VAL:CA   | 42:c:70:GLU:OE1   | 2.69                     | 0.41              |
| 43:d:55:U:H2'    | 43:d:56:G:C8      | 2.56                     | 0.41              |
| 46:g:57:VAL:O    | 46:g:58:ASP:C     | 2.62                     | 0.41              |
| 46:g:62:LYS:HE2  | 46:g:62:LYS:HB2   | 1.87                     | 0.41              |
| 47:h:53:HIS:CD2  | 47:h:218:PRO:O    | 2.74                     | 0.41              |
| 47:h:220:VAL:CG2 | 47:h:225:MET:HE3  | 2.51                     | 0.41              |
| 49:j:108:ASP:OD1 | 49:j:173:GLN:HA   | 2.21                     | 0.41              |
| 50:k:7:GLU:CG    | 50:k:27:LYS:NZ    | 2.84                     | 0.41              |
| 53:n:136:ILE:HA  | 53:n:141:ILE:CG2  | 2.51                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 53:n:141:ILE:HD11 | 53:n:146:VAL:CG1    | 2.50                     | 0.41              |
| 54:o:30:ARG:CZ    | 60:u:62:PRO:HB3     | 2.50                     | 0.41              |
| 55:p:45:HIS:HA    | 55:p:50:LEU:HD13    | 2.01                     | 0.41              |
| 58:s:49:ASP:OD1   | 58:s:121:LYS:NZ     | 2.54                     | 0.41              |
| 60:u:95:LEU:HD13  | 60:u:100:ILE:CD1    | 2.51                     | 0.41              |
| 60:u:123:ARG:HG3  | 60:u:143:GLU:OE2    | 2.21                     | 0.41              |
| 61:v:31:PHE:CZ    | 61:v:110:GLU:HG3    | 2.56                     | 0.41              |
| 62:w:17:ARG:O     | 62:w:21:PHE:HD2     | 2.04                     | 0.41              |
| 62:w:24:MET:CG    | 62:w:44:LEU:HD12    | 2.51                     | 0.41              |
| 62:w:33:ILE:HG13  | 62:w:112:TYR:HD1    | 1.83                     | 0.41              |
| 62:w:45:ARG:HB3   | 62:w:45:ARG:CZ      | 2.50                     | 0.41              |
| 65:z:66:ASN:OD1   | 65:z:70:ARG:NE      | 2.54                     | 0.41              |
| 1:0:13:ARG:NH2    | 65:z:97:ASP:CG      | 2.79                     | 0.41              |
| 9:9:96:PHE:O      | 9:9:125:ARG:NH1     | 2.54                     | 0.41              |
| 9:9:96:PHE:HB3    | 9:9:125:ARG:HH11    | 1.86                     | 0.41              |
| 10:A:25:C:C4      | 10:A:26:G:C8        | 3.09                     | 0.41              |
| 11:AA:803:ALA:HB2 | 11:AA:1094:VAL:HG21 | 2.03                     | 0.41              |
| 12:AB:4:TRP:CZ3   | 12:AB:93:ILE:HG13   | 2.56                     | 0.41              |
| 12:AB:95:GLN:C    | 12:AB:96:LEU:HD12   | 2.46                     | 0.41              |
| 12:AB:106:ASP:O   | 12:AB:109:THR:OG1   | 2.38                     | 0.41              |
| 14:AE:438:GLU:OE2 | 14:AE:481:ARG:NH1   | 2.44                     | 0.41              |
| 14:AE:649:LYS:NZ  | 14:AE:652:GLU:OE1   | 2.38                     | 0.41              |
| 14:AE:800:LEU:HB3 | 14:AE:920:ALA:HB1   | 2.02                     | 0.41              |
| 10:B:22:G:HO2'    | 10:B:23:C:P         | 2.43                     | 0.41              |
| 10:B:25:C:C4      | 10:B:26:G:C8        | 3.09                     | 0.41              |
| 10:B:68:C:C4      | 10:B:69:C:C5        | 3.08                     | 0.41              |
| 17:D:104:G:C2     | 17:D:105:G:C5       | 3.09                     | 0.41              |
| 17:D:114:U:H2'    | 17:D:115:G:C8       | 2.56                     | 0.41              |
| 17:D:218:U:H2'    | 17:D:219:U:O4'      | 2.20                     | 0.41              |
| 17:D:982:U:H4'    | 17:D:983:A:O4'      | 2.21                     | 0.41              |
| 17:D:1064:G:O2'   | 17:D:1190:G:N2      | 2.53                     | 0.41              |
| 17:D:1227:A:OP2   | 37:X:110:LYS:HE3    | 2.20                     | 0.41              |
| 17:D:1318:A:OP1   | 36:W:7:LYS:NZ       | 2.52                     | 0.41              |
| 17:D:1411:C:H2'   | 17:D:1412:C:C6      | 2.56                     | 0.41              |
| 17:D:1512:U:H2'   | 17:D:1513:A:H8      | 1.85                     | 0.41              |
| 20:G:47:VAL:N     | 20:G:48:PRO:HD2     | 2.35                     | 0.41              |
| 20:G:187:VAL:HG11 | 20:G:193:PRO:HB3    | 2.02                     | 0.41              |
| 20:G:187:VAL:N    | 20:G:200:ILE:O      | 2.40                     | 0.41              |
| 22:I:72:ARG:CD    | 22:I:75:ILE:HB      | 2.51                     | 0.41              |
| 23:J:138:SER:C    | 23:J:182:PHE:CE2    | 2.99                     | 0.41              |
| 23:J:188:ARG:NH2  | 23:J:195:ILE:HG13   | 2.36                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:M:35:LYS:CE     | 26:M:38:THR:OG1    | 2.69                     | 0.41              |
| 26:M:66:LEU:HA     | 26:M:66:LEU:HD12   | 1.84                     | 0.41              |
| 28:O:35:LEU:HD21   | 28:O:45:ARG:HG2    | 2.03                     | 0.41              |
| 29:P:85:ASP:CA     | 29:P:88:MET:HE1    | 2.42                     | 0.41              |
| 30:Q:21:ALA:HA     | 30:Q:34:ILE:HD13   | 2.02                     | 0.41              |
| 30:Q:87:LYS:CG     | 30:Q:113:VAL:CG2   | 2.89                     | 0.41              |
| 30:Q:94:GLU:O      | 30:Q:94:GLU:OE2    | 2.39                     | 0.41              |
| 39:Z:20:VAL:O      | 39:Z:20:VAL:CG1    | 2.65                     | 0.41              |
| 40:a:16:C:C4'      | 48:i:15:MET:CE     | 2.99                     | 0.41              |
| 40:a:689:A:H2'     | 40:a:690:G:H8      | 1.86                     | 0.41              |
| 40:a:708:G:H2'     | 40:a:709:U:H6      | 1.86                     | 0.41              |
| 40:a:833:A:OP2     | 60:u:39:LYS:NZ     | 2.49                     | 0.41              |
| 40:a:945:A:C4      | 40:a:2448:A:C2     | 3.09                     | 0.41              |
| 40:a:1322:A:C4     | 40:a:1323:C:C6     | 3.08                     | 0.41              |
| 40:a:1351:C:H2'    | 40:a:1352:U:O4'    | 2.21                     | 0.41              |
| 40:a:1571:A:H2'    | 40:a:1572:A:H8     | 1.86                     | 0.41              |
| 40:a:1589:U:C2     | 40:a:1590:A:C8     | 3.09                     | 0.41              |
| 40:a:2357:G:OP1    | 41:b:20:ARG:CZ     | 2.68                     | 0.41              |
| 40:a:2483:C:H1'    | 61:v:51:ARG:CZ     | 2.51                     | 0.41              |
| 40:a:2728:U:H5'    | 59:t:70:ARG:HH22   | 1.85                     | 0.41              |
| 51:l:171:ASP:OD1   | 51:l:172:ALA:N     | 2.53                     | 0.41              |
| 57:r:110:VAL:HG21  | 57:r:114:GLU:OE1   | 2.21                     | 0.41              |
| 58:s:53:TYR:HD1    | 58:s:121:LYS:HB3   | 1.85                     | 0.41              |
| 58:s:99:ARG:O      | 58:s:100:VAL:C     | 2.63                     | 0.41              |
| 59:t:1:MET:HE3     | 59:t:32:TYR:CB     | 2.50                     | 0.41              |
| 59:t:24:VAL:O      | 59:t:24:VAL:HG13   | 2.20                     | 0.41              |
| 60:u:96:LYS:HG2    | 60:u:102:GLY:O     | 2.21                     | 0.41              |
| 60:u:101:ILE:HG13  | 60:u:102:GLY:N     | 2.36                     | 0.41              |
| 5:4:78:GLN:OE1     | 5:4:88:HIS:HB3     | 2.21                     | 0.40              |
| 9:9:38:MET:SD      | 9:9:41:LEU:HD12    | 2.61                     | 0.40              |
| 11:AA:148:GLN:NE2  | 11:AA:535:PRO:O    | 2.40                     | 0.40              |
| 11:AA:836:LEU:HD21 | 11:AA:921:PRO:HD3  | 2.02                     | 0.40              |
| 12:AB:112:PRO:HA   | 12:AB:133:PRO:HD2  | 2.03                     | 0.40              |
| 13:AD:44:ARG:HA    | 13:AD:183:ILE:HD12 | 2.03                     | 0.40              |
| 14:AE:438:GLU:HG3  | 14:AE:485:MET:HE1  | 2.03                     | 0.40              |
| 14:AE:591:ILE:HG23 | 14:AE:592:VAL:HG13 | 2.03                     | 0.40              |
| 17:D:105:G:H2'     | 17:D:106:C:C6      | 2.56                     | 0.40              |
| 17:D:502:A:H2'     | 17:D:503:C:H6      | 1.86                     | 0.40              |
| 17:D:570:G:H1'     | 17:D:820:U:C4      | 2.56                     | 0.40              |
| 17:D:1228:C:OP1    | 37:X:107:ARG:CZ    | 2.69                     | 0.40              |
| 20:G:94:HIS:O      | 20:G:95:ARG:C      | 2.64                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:G:138:THR:O   | 20:G:142:GLU:HG2 | 2.21                     | 0.40              |
| 20:G:185:ALA:O   | 20:G:200:ILE:N   | 2.54                     | 0.40              |
| 21:H:303:LEU:O   | 21:H:305:HIS:HA  | 2.21                     | 0.40              |
| 22:I:6:HIS:CD2   | 22:I:9:GLY:H     | 2.39                     | 0.40              |
| 22:I:8:ASN:O     | 22:I:12:LEU:HD23 | 2.21                     | 0.40              |
| 22:I:132:ARG:HA  | 22:I:135:LYS:HG2 | 2.04                     | 0.40              |
| 22:I:147:LYS:CE  | 22:I:204:LYS:C   | 2.94                     | 0.40              |
| 25:L:9:MET:CE    | 25:L:86:ARG:HG2  | 2.51                     | 0.40              |
| 29:P:47:GLU:N    | 29:P:47:GLU:CD   | 2.79                     | 0.40              |
| 31:R:27:CYS:CB   | 31:R:30:LYS:HE2  | 2.47                     | 0.40              |
| 34:U:3:THR:HG22  | 34:U:22:ALA:O    | 2.21                     | 0.40              |
| 35:V:11:ARG:HD3  | 35:V:57:ASP:C    | 2.46                     | 0.40              |
| 38:Y:91:LYS:HZ3  | 38:Y:97:VAL:HG21 | 1.82                     | 0.40              |
| 40:a:30:G:H2'    | 40:a:31:C:C6     | 2.55                     | 0.40              |
| 40:a:126:A:O5'   | 52:m:19:ARG:HG3  | 2.21                     | 0.40              |
| 40:a:241:A:N1    | 40:a:255:A:H5''  | 2.36                     | 0.40              |
| 40:a:397:U:H2'   | 40:a:398:C:C6    | 2.56                     | 0.40              |
| 40:a:1048:A:C5   | 40:a:1049:C:C5   | 3.09                     | 0.40              |
| 40:a:1144:A:C6   | 40:a:1145:C:C4   | 3.09                     | 0.40              |
| 40:a:1406:U:C2   | 40:a:1407:G:N7   | 2.89                     | 0.40              |
| 40:a:1746:A:H2'  | 40:a:1747:U:C6   | 2.56                     | 0.40              |
| 40:a:1792:G:C5'  | 47:h:204:VAL:CG2 | 2.99                     | 0.40              |
| 40:a:1827:U:H2'  | 40:a:1828:G:O4'  | 2.20                     | 0.40              |
| 40:a:1858:A:C2   | 40:a:1885:A:C1'  | 3.04                     | 0.40              |
| 40:a:1944:U:C5   | 40:a:1955:U:C2   | 3.09                     | 0.40              |
| 40:a:1953:A:H2   | 40:a:2549:G:N3   | 2.18                     | 0.40              |
| 40:a:2065:C:C2   | 40:a:2066:C:C6   | 3.09                     | 0.40              |
| 40:a:2223:G:OP1  | 47:h:171:TYR:OH  | 2.37                     | 0.40              |
| 40:a:2759:G:H1'  | 55:p:35:ARG:HH22 | 1.86                     | 0.40              |
| 42:c:3:ARG:HD2   | 42:c:30:LEU:CD1  | 2.51                     | 0.40              |
| 45:f:5:ILE:HG22  | 45:f:6:LYS:N     | 2.36                     | 0.40              |
| 45:f:25:LEU:HD23 | 45:f:25:LEU:C    | 2.46                     | 0.40              |
| 50:k:8:LYS:HA    | 50:k:24:THR:HA   | 2.02                     | 0.40              |
| 51:l:97:ASN:CG   | 51:l:100:MET:HE2 | 2.45                     | 0.40              |
| 53:n:8:TYR:O     | 53:n:13:VAL:HG23 | 2.20                     | 0.40              |
| 55:p:80:THR:HG23 | 55:p:81:GLU:N    | 2.36                     | 0.40              |
| 55:p:137:ASP:OD2 | 55:p:140:VAL:N   | 2.45                     | 0.40              |
| 55:p:149:ARG:CZ  | 55:p:154:PRO:CD  | 2.99                     | 0.40              |
| 59:t:20:MET:CB   | 59:t:44:LYS:HE2  | 2.51                     | 0.40              |
| 59:t:61:VAL:HG11 | 59:t:112:PHE:CE2 | 2.56                     | 0.40              |
| 2:1:85:ILE:HG13  | 2:1:85:ILE:O     | 2.19                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:3:47:LYS:NZ     | 40:a:482:A:H5''  | 2.37                     | 0.40              |
| 4:3:86:ARG:NH2    | 4:3:95:PHE:CB    | 2.84                     | 0.40              |
| 8:7:10:U:O2       | 8:7:10:U:H3'     | 2.21                     | 0.40              |
| 8:7:19:U:C6       | 8:7:19:U:C3'     | 3.04                     | 0.40              |
| 9:9:6:GLN:HA      | 9:9:9:GLN:HE21   | 1.85                     | 0.40              |
| 9:9:98:GLU:CB     | 9:9:101:LYS:HZ1  | 2.34                     | 0.40              |
| 9:9:123:ILE:O     | 9:9:123:ILE:CG2  | 2.68                     | 0.40              |
| 12:AB:8:TYR:C     | 12:AB:76:SER:HB3 | 2.46                     | 0.40              |
| 12:AB:72:THR:HG22 | 12:AB:73:ARG:H   | 1.86                     | 0.40              |
| 10:B:9:G:H5''     | 10:B:11:A:OP2    | 2.21                     | 0.40              |
| 16:C:38:LYS:NZ    | 17:D:718:A:C6    | 2.79                     | 0.40              |
| 16:C:70:TYR:CD2   | 17:D:674:G:H4'   | 2.55                     | 0.40              |
| 17:D:107:G:C6     | 17:D:108:G:C4    | 3.09                     | 0.40              |
| 17:D:296:U:O2'    | 17:D:556:C:O2    | 2.34                     | 0.40              |
| 17:D:619:U:C1'    | 23:J:128:ARG:NH1 | 2.85                     | 0.40              |
| 18:E:43:ASP:CG    | 18:E:46:ALA:HB3  | 2.46                     | 0.40              |
| 20:G:90:PHE:CD2   | 20:G:154:MET:SD  | 3.15                     | 0.40              |
| 20:G:137:ARG:HG3  | 20:G:138:THR:N   | 2.36                     | 0.40              |
| 25:L:51:ILE:CG2   | 25:L:86:ARG:HH21 | 2.34                     | 0.40              |
| 33:T:3:LEU:HB2    | 33:T:35:GLN:OE1  | 2.22                     | 0.40              |
| 34:U:69:ASP:OD1   | 34:U:69:ASP:C    | 2.63                     | 0.40              |
| 37:X:13:LYS:CE    | 37:X:17:ILE:HG21 | 2.51                     | 0.40              |
| 38:Y:28:GLY:HA3   | 38:Y:32:VAL:HB   | 2.03                     | 0.40              |
| 40:a:181:A:H2'    | 40:a:182:A:C8    | 2.56                     | 0.40              |
| 40:a:244:A:H2'    | 40:a:245:G:O4'   | 2.21                     | 0.40              |
| 40:a:638:G:H2'    | 40:a:639:U:C6    | 2.56                     | 0.40              |
| 40:a:706:A:C2     | 40:a:707:G:H1'   | 2.57                     | 0.40              |
| 40:a:752:A:P      | 52:m:1:MET:HE1   | 2.62                     | 0.40              |
| 40:a:1177:G:O2'   | 40:a:1178:C:O4'  | 2.39                     | 0.40              |
| 40:a:1248:G:O2'   | 65:z:3:ARG:HA    | 2.21                     | 0.40              |
| 40:a:1294:U:C4    | 40:a:1295:C:C5   | 3.10                     | 0.40              |
| 40:a:1509:A:HO2'  | 40:a:1510:G:P    | 2.45                     | 0.40              |
| 40:a:1548:A:H2'   | 40:a:1549:A:C8   | 2.56                     | 0.40              |
| 40:a:1607:C:H4'   | 40:a:1608:A:O5'  | 2.21                     | 0.40              |
| 40:a:1824:G:O5'   | 47:h:52:ARG:NH1  | 2.53                     | 0.40              |
| 40:a:1996:C:H4'   | 49:j:128:ARG:NH1 | 2.35                     | 0.40              |
| 40:a:2000:C:OP1   | 62:w:5:LYS:NZ    | 2.38                     | 0.40              |
| 40:a:2049:G:H21   | 49:j:161:MET:CE  | 2.33                     | 0.40              |
| 40:a:2216:G:H2'   | 40:a:2217:G:C8   | 2.57                     | 0.40              |
| 40:a:2393:U:H2'   | 40:a:2394:C:C6   | 2.56                     | 0.40              |
| 40:a:2422:C:C4    | 40:a:2424:C:C4   | 3.09                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:a:2627:G:H2'    | 40:a:2628:C:C6     | 2.56                     | 0.40              |
| 40:a:2821:A:H4'    | 49:j:167:ASN:ND2   | 2.36                     | 0.40              |
| 40:a:2839:G:C4     | 40:a:2840:C:C6     | 3.09                     | 0.40              |
| 41:b:58:THR:O      | 41:b:58:THR:HG23   | 2.21                     | 0.40              |
| 47:h:137:VAL:HA    | 47:h:164:ILE:HG23  | 2.03                     | 0.40              |
| 47:h:163:GLN:HB3   | 47:h:175:ARG:HB3   | 2.02                     | 0.40              |
| 48:i:34:SER:OG     | 48:i:36:GLU:HG2    | 2.20                     | 0.40              |
| 55:p:149:ARG:NH1   | 55:p:154:PRO:CG    | 2.84                     | 0.40              |
| 57:r:76:GLU:OE2    | 57:r:142:VAL:HA    | 2.21                     | 0.40              |
| 59:t:1:MET:HE1     | 59:t:32:TYR:HB3    | 2.03                     | 0.40              |
| 59:t:7:MET:CE      | 59:t:20:MET:HB2    | 2.51                     | 0.40              |
| 61:v:135:VAL:HG12  | 61:v:136:MET:CE    | 2.50                     | 0.40              |
| 62:w:47:VAL:C      | 62:w:50:PRO:HD2    | 2.47                     | 0.40              |
| 64:y:48:ILE:HD11   | 64:y:101:ARG:NH1   | 2.36                     | 0.40              |
| 3:2:50:LEU:HD23    | 44:e:26:PHE:CE1    | 2.56                     | 0.40              |
| 5:4:77:VAL:HG21    | 5:4:79:ARG:HH21    | 1.86                     | 0.40              |
| 9:9:122:GLN:HG2    | 9:9:123:ILE:HG22   | 2.04                     | 0.40              |
| 10:A:1:C:C5        | 10:A:2:G:N7        | 2.89                     | 0.40              |
| 10:A:5:G:C2'       | 10:A:6:G:H5'       | 2.50                     | 0.40              |
| 10:A:33:U:H5''     | 26:M:84:THR:CG2    | 2.50                     | 0.40              |
| 11:AA:176:ILE:HD12 | 11:AA:184:LEU:HD23 | 2.04                     | 0.40              |
| 11:AA:1105:SER:HB2 | 14:AE:731:ARG:HB3  | 2.03                     | 0.40              |
| 12:AB:2:GLN:HA     | 12:AB:59:PHE:O     | 2.21                     | 0.40              |
| 12:AB:32:MET:O     | 12:AB:50:LEU:HD12  | 2.22                     | 0.40              |
| 12:AB:154:VAL:CG2  | 12:AB:158:GLU:HB2  | 2.51                     | 0.40              |
| 17:D:262:A:C4      | 17:D:263:A:C8      | 3.10                     | 0.40              |
| 17:D:511:C:O3'     | 23:J:44:ARG:NH1    | 2.53                     | 0.40              |
| 17:D:562:U:O3'     | 31:R:12:ARG:HD2    | 2.20                     | 0.40              |
| 17:D:624:C:H2'     | 17:D:625:U:O4'     | 2.22                     | 0.40              |
| 17:D:1061:G:C6     | 17:D:1197:A:C6     | 3.09                     | 0.40              |
| 17:D:1367:C:O3'    | 28:O:116:VAL:HG22  | 2.22                     | 0.40              |
| 17:D:1372:U:H2'    | 17:D:1373:G:O4'    | 2.22                     | 0.40              |
| 18:E:45:ALA:O      | 18:E:48:GLN:NE2    | 2.49                     | 0.40              |
| 20:G:161:LEU:HD13  | 20:G:176:ALA:HB2   | 2.03                     | 0.40              |
| 21:H:42:LEU:HD23   | 21:H:81:GLU:HB3    | 2.04                     | 0.40              |
| 24:K:82:GLN:OE1    | 24:K:147:MET:SD    | 2.78                     | 0.40              |
| 24:K:133:PRO:HA    | 24:K:136:VAL:HG12  | 2.02                     | 0.40              |
| 27:N:83:LEU:HD23   | 35:V:36:LYS:CD     | 2.52                     | 0.40              |
| 28:O:91:ASP:C      | 28:O:92:GLU:OE2    | 2.64                     | 0.40              |
| 31:R:7:LEU:HD21    | 31:R:12:ARG:HH21   | 1.82                     | 0.40              |
| 34:U:18:GLN:CD     | 34:U:35:ARG:HE     | 2.30                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:X:55:THR:CG2    | 37:X:59:GLU:OE2    | 2.69                     | 0.40              |
| 38:Y:9:LYS:O       | 38:Y:10:LEU:HG     | 2.21                     | 0.40              |
| 38:Y:100:ILE:HG13  | 38:Y:139:VAL:HB    | 2.02                     | 0.40              |
| 40:a:1005:C:H1'    | 40:a:1012:U:N3     | 2.37                     | 0.40              |
| 40:a:1059:G:C6     | 40:a:1080:A:N1     | 2.90                     | 0.40              |
| 40:a:1816:C:H3'    | 47:h:62:TYR:CE1    | 2.57                     | 0.40              |
| 40:a:1881:C:C4     | 40:a:1882:U:C5     | 3.09                     | 0.40              |
| 40:a:1923:U:H2'    | 40:a:1923:U:OP2    | 2.21                     | 0.40              |
| 40:a:2314:A:O2'    | 53:n:155:THR:CG2   | 2.69                     | 0.40              |
| 40:a:2364:C:O2'    | 41:b:58:THR:HG21   | 2.21                     | 0.40              |
| 40:a:2520:C:O2'    | 40:a:2521:C:H5'    | 2.20                     | 0.40              |
| 40:a:2839:G:H2'    | 40:a:2840:C:H6     | 1.87                     | 0.40              |
| 40:a:2851:A:H2'    | 40:a:2852:G:C8     | 2.56                     | 0.40              |
| 41:b:17:GLU:OE1    | 41:b:19:LYS:HD3    | 2.21                     | 0.40              |
| 45:f:34:HIS:CD2    | 45:f:36:VAL:CG2    | 3.04                     | 0.40              |
| 47:h:84:ASP:OD2    | 47:h:91:ILE:HD11   | 2.21                     | 0.40              |
| 47:h:183:LYS:HZ2   | 47:h:268:VAL:HG22  | 1.86                     | 0.40              |
| 49:j:55:LYS:HZ1    | 49:j:60:VAL:CA     | 2.34                     | 0.40              |
| 49:j:184:ARG:HH22  | 64:y:7:GLN:CD      | 2.26                     | 0.40              |
| 50:k:12:VAL:HG12   | 50:k:50:LYS:O      | 2.22                     | 0.40              |
| 58:s:114:LEU:O     | 58:s:118:MET:HG3   | 2.21                     | 0.40              |
| 59:t:80:ASP:OD1    | 64:y:68:GLU:OE2    | 2.39                     | 0.40              |
| 62:w:98:LEU:HD12   | 62:w:114:GLU:OE2   | 2.21                     | 0.40              |
| 64:y:4:ILE:O       | 64:y:8:LEU:HD13    | 2.21                     | 0.40              |
| 1:0:13:ARG:C       | 1:0:14:VAL:HG13    | 2.46                     | 0.40              |
| 2:1:93:ALA:HB2     | 40:a:1614:A:C2     | 2.57                     | 0.40              |
| 3:2:6:ARG:NH2      | 3:2:10:VAL:CG2     | 2.84                     | 0.40              |
| 7:6:2:DC:H6        | 7:6:2:DC:H2'       | 1.76                     | 0.40              |
| 9:9:59:LEU:HD22    | 9:9:62:ARG:CD      | 2.51                     | 0.40              |
| 10:A:16:C:O2       | 10:A:16:C:H2'      | 2.21                     | 0.40              |
| 11:AA:519:ASN:HD21 | 11:AA:796:LEU:HD23 | 1.87                     | 0.40              |
| 12:AB:2:GLN:N      | 12:AB:60:ASP:OD1   | 2.54                     | 0.40              |
| 12:AB:51:PHE:CD2   | 12:AB:54:TYR:HD2   | 2.39                     | 0.40              |
| 12:AB:158:GLU:HA   | 12:AB:162:LEU:HA   | 2.04                     | 0.40              |
| 13:AC:57:THR:HG23  | 13:AC:158:ARG:HH21 | 1.86                     | 0.40              |
| 14:AE:291:ILE:HD13 | 14:AE:291:ILE:HA   | 1.85                     | 0.40              |
| 10:B:70:G:H3'      | 10:B:71:C:H5''     | 2.04                     | 0.40              |
| 17:D:74:A:C4       | 17:D:75:G:C8       | 3.09                     | 0.40              |
| 17:D:436:C:N3      | 17:D:437:U:C5      | 2.89                     | 0.40              |
| 17:D:582:C:C2      | 17:D:583:A:C8      | 3.10                     | 0.40              |
| 17:D:680:C:C2      | 17:D:681:A:C8      | 3.09                     | 0.40              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 17:D:958:A:H5'   | 36:W:55:ARG:HH12   | 1.86                     | 0.40              |
| 17:D:983:A:C2    | 17:D:984:C:C6      | 3.10                     | 0.40              |
| 17:D:1141:C:O2'  | 17:D:1142:G:P      | 2.79                     | 0.40              |
| 17:D:1326:U:H2'  | 17:D:1327:C:C6     | 2.56                     | 0.40              |
| 17:D:1499:A:H3'  | 17:D:1499:A:OP2    | 2.22                     | 0.40              |
| 18:E:27:MET:SD   | 18:E:31:PHE:CE2    | 3.15                     | 0.40              |
| 18:E:28:MET:HE3  | 18:E:28:MET:HB3    | 1.94                     | 0.40              |
| 18:E:59:ASP:OD1  | 18:E:76:LYS:HE2    | 2.21                     | 0.40              |
| 19:F:12:PHE:O    | 19:F:16:LEU:HG     | 2.21                     | 0.40              |
| 22:I:30:ALA:O    | 32:S:65:ARG:NH2    | 2.54                     | 0.40              |
| 22:I:47:LEU:HD22 | 22:I:76:VAL:HG22   | 2.03                     | 0.40              |
| 22:I:135:LYS:HG3 | 22:I:136:ARG:N     | 2.35                     | 0.40              |
| 22:I:135:LYS:HA  | 22:I:138:VAL:HG12  | 2.04                     | 0.40              |
| 27:N:28:PRO:HD3  | 27:N:58:GLU:OE1    | 2.21                     | 0.40              |
| 28:O:7:TYR:CG    | 28:O:8:GLY:N       | 2.90                     | 0.40              |
| 30:Q:36:ASP:OD1  | 30:Q:40:ASN:N      | 2.53                     | 0.40              |
| 31:R:4:VAL:CG1   | 31:R:5:ASN:N       | 2.83                     | 0.40              |
| 31:R:59:ASN:OD1  | 31:R:59:ASN:C      | 2.62                     | 0.40              |
| 32:S:37:SER:O    | 32:S:41:ARG:HG3    | 2.22                     | 0.40              |
| 35:V:26:GLU:OE2  | 35:V:39:LYS:C      | 2.65                     | 0.40              |
| 37:X:36:ALA:HB3  | 37:X:59:GLU:HG2    | 2.03                     | 0.40              |
| 40:a:48:G:C2     | 40:a:178:G:C6      | 3.09                     | 0.40              |
| 40:a:409:G:H2'   | 40:a:410:G:C8      | 2.55                     | 0.40              |
| 40:a:1398:C:H2'  | 40:a:1399:C:H6     | 1.86                     | 0.40              |
| 40:a:1709:U:C2   | 40:a:1710:G:C8     | 3.10                     | 0.40              |
| 40:a:2680:U:H1'  | 49:j:192:ALA:CB    | 2.52                     | 0.40              |
| 43:d:8:C:O2'     | 63:x:40:ILE:HD13   | 2.21                     | 0.40              |
| 43:d:47:C:C4     | 43:d:48:U:C5       | 3.09                     | 0.40              |
| 49:j:176:ASP:OD2 | 49:j:176:ASP:C     | 2.65                     | 0.40              |
| 50:k:7:GLU:OE2   | 50:k:27:LYS:N      | 2.50                     | 0.40              |
| 50:k:26:ASN:OD1  | 50:k:28:ARG:NH1    | 2.54                     | 0.40              |
| 51:l:148:ILE:O   | 51:l:169:VAL:HA    | 2.21                     | 0.40              |
| 52:m:12:ARG:HG3  | 52:m:44:VAL:HG21   | 2.03                     | 0.40              |
| 52:m:42:LEU:N    | 52:m:42:LEU:HD12   | 2.36                     | 0.40              |
| 53:n:30:ARG:O    | 53:n:159:THR:HG23  | 2.22                     | 0.40              |
| 61:v:115:GLU:HA  | 61:v:118:LYS:HE2   | 2.02                     | 0.40              |
| 2:1:32:ALA:O     | 2:1:36:LEU:CD1     | 2.70                     | 0.40              |
| 4:3:86:ARG:CZ    | 4:3:95:PHE:CD2     | 3.04                     | 0.40              |
| 6:5:25:DA:N3     | 7:6:5:DG:N2        | 2.68                     | 0.40              |
| 8:7:37:G:P       | 11:AA:688:GLN:HE22 | 2.45                     | 0.40              |
| 9:9:43:LYS:HA    | 9:9:46:ARG:NH2     | 2.35                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:A:70:G:H3'      | 10:A:71:C:H5''     | 2.04                     | 0.40              |
| 11:AA:95:PRO:HB3   | 11:AA:123:TYR:HE1  | 1.87                     | 0.40              |
| 11:AA:1069:ARG:NH2 | 11:AA:1114:GLU:OE2 | 2.44                     | 0.40              |
| 12:AB:146:ILE:H    | 12:AB:146:ILE:HD12 | 1.86                     | 0.40              |
| 10:B:9:G:O2'       | 10:B:45:G:H2'      | 2.20                     | 0.40              |
| 16:C:51:TYR:HA     | 16:C:54:GLN:NE2    | 2.36                     | 0.40              |
| 16:C:73:ARG:NH1    | 30:Q:113:VAL:CB    | 2.82                     | 0.40              |
| 17:D:9:G:OP2       | 24:K:126:LYS:HD2   | 2.21                     | 0.40              |
| 17:D:19:A:C6       | 17:D:20:U:C4       | 3.10                     | 0.40              |
| 17:D:105:G:C6      | 17:D:106:C:C4      | 3.10                     | 0.40              |
| 17:D:333:U:OP1     | 18:E:2:ALA:N       | 2.55                     | 0.40              |
| 17:D:407:U:O4'     | 23:J:116:GLN:OE1   | 2.39                     | 0.40              |
| 17:D:427:U:OP2     | 17:D:428:G:O2'     | 2.31                     | 0.40              |
| 17:D:567:G:H2'     | 17:D:568:G:O4'     | 2.21                     | 0.40              |
| 17:D:953:G:O6      | 37:X:103:LYS:HE2   | 2.22                     | 0.40              |
| 17:D:1095:U:H2'    | 17:D:1096:C:C6     | 2.57                     | 0.40              |
| 17:D:1227:A:C8     | 37:X:116:ILE:HD11  | 2.56                     | 0.40              |
| 20:G:17:GLY:C      | 21:H:43:LYS:HD2    | 2.46                     | 0.40              |
| 25:L:1:MET:HE2     | 25:L:66:ALA:C      | 2.47                     | 0.40              |
| 25:L:3:HIS:CD2     | 25:L:95:ALA:HA     | 2.56                     | 0.40              |
| 25:L:4:TYR:CD2     | 25:L:91:ARG:HD2    | 2.57                     | 0.40              |
| 25:L:11:HIS:HE1    | 25:L:13:ASP:OD2    | 2.05                     | 0.40              |
| 27:N:50:LYS:HA     | 27:N:50:LYS:CE     | 2.52                     | 0.40              |
| 32:S:63:ARG:HB3    | 32:S:68:GLY:HA2    | 2.04                     | 0.40              |
| 36:W:34:TRP:O      | 36:W:36:ARG:N      | 2.54                     | 0.40              |
| 37:X:65:VAL:CG2    | 37:X:66:GLU:OE1    | 2.69                     | 0.40              |
| 38:Y:55:PRO:C      | 38:Y:71:LYS:CE     | 2.95                     | 0.40              |
| 38:Y:99:LYS:HD3    | 38:Y:99:LYS:HA     | 1.86                     | 0.40              |
| 38:Y:102:ARG:NH2   | 38:Y:139:VAL:HG11  | 2.36                     | 0.40              |
| 40:a:78:U:P        | 44:e:4:LYS:HZ1     | 2.44                     | 0.40              |
| 40:a:216:A:C8      | 40:a:432:A:C6      | 3.10                     | 0.40              |
| 40:a:392:U:N3      | 40:a:393:C:C5      | 2.90                     | 0.40              |
| 40:a:545:U:O2'     | 40:a:546:U:O3'     | 2.39                     | 0.40              |
| 40:a:1196:C:H2'    | 40:a:1197:G:O4'    | 2.22                     | 0.40              |
| 40:a:1469:A:OP2    | 40:a:1522:A:N6     | 2.52                     | 0.40              |
| 40:a:1494:A:H2'    | 40:a:1495:A:C8     | 2.56                     | 0.40              |
| 40:a:1589:U:O2'    | 40:a:1590:A:P      | 2.79                     | 0.40              |
| 40:a:2422:C:N4     | 40:a:2424:C:N4     | 2.70                     | 0.40              |
| 40:a:2511:U:O4'    | 49:j:130:GLN:OE1   | 2.39                     | 0.40              |
| 40:a:2549:G:C2     | 40:a:2550:G:C5     | 3.10                     | 0.40              |
| 41:b:55:ARG:NE     | 41:b:55:ARG:CA     | 2.84                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 46:g:2:LYS:HB2   | 46:g:5:ILE:CD1   | 2.52                     | 0.40              |
| 47:h:74:ILE:HG22 | 47:h:96:TYR:HD1  | 1.86                     | 0.40              |
| 49:j:11:MET:SD   | 49:j:12:THR:N    | 2.94                     | 0.40              |
| 49:j:55:LYS:HD3  | 49:j:56:LYS:N    | 2.36                     | 0.40              |
| 50:k:19:HIS:ND1  | 50:k:41:PRO:HD3  | 2.36                     | 0.40              |
| 53:n:49:LEU:N    | 53:n:49:LEU:HD12 | 2.37                     | 0.40              |
| 53:n:61:SER:O    | 53:n:63:GLN:N    | 2.54                     | 0.40              |
| 61:v:73:ILE:HD13 | 61:v:93:VAL:HG13 | 2.04                     | 0.40              |
| 61:v:105:MET:HG2 | 61:v:117:PHE:HZ  | 1.86                     | 0.40              |
| 61:v:106:ASP:OD1 | 61:v:106:ASP:C   | 2.64                     | 0.40              |
| 63:x:4:LYS:O     | 63:x:8:ILE:HG12  | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | 0     | 101/103 (98%)   | 97 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 2   | 1     | 108/110 (98%)   | 107 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 3   | 2     | 92/100 (92%)    | 87 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 4   | 3     | 101/104 (97%)   | 98 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 5   | 4     | 92/94 (98%)     | 89 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 9   | 9     | 146/165 (88%)   | 101 (69%)  | 42 (29%) | 3 (2%)   | 5           | 28  |
| 11  | AA    | 1312/1342 (98%) | 1199 (91%) | 112 (8%) | 1 (0%)   | 48          | 82  |
| 12  | AB    | 159/162 (98%)   | 109 (69%)  | 45 (28%) | 5 (3%)   | 3           | 21  |
| 13  | AC    | 217/329 (66%)   | 203 (94%)  | 12 (6%)  | 2 (1%)   | 14          | 49  |
| 13  | AD    | 214/329 (65%)   | 198 (92%)  | 16 (8%)  | 0        | 100         | 100 |
| 14  | AE    | 1331/1407 (95%) | 1210 (91%) | 115 (9%) | 6 (0%)   | 24          | 63  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 15  | AF    | 80/91 (88%)   | 77 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 16  | C     | 64/75 (85%)   | 63 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 18  | E     | 84/87 (97%)   | 83 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 19  | F     | 68/71 (96%)   | 68 (100%) | 0        | 0        | 100         | 100 |
| 20  | G     | 223/241 (92%) | 212 (95%) | 10 (4%)  | 1 (0%)   | 30          | 67  |
| 21  | H     | 255/557 (46%) | 182 (71%) | 66 (26%) | 7 (3%)   | 4           | 24  |
| 22  | I     | 206/233 (88%) | 193 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 23  | J     | 203/206 (98%) | 201 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 24  | K     | 154/167 (92%) | 145 (94%) | 8 (5%)   | 1 (1%)   | 21          | 58  |
| 25  | L     | 102/135 (76%) | 97 (95%)  | 4 (4%)   | 1 (1%)   | 12          | 47  |
| 26  | M     | 149/179 (83%) | 140 (94%) | 8 (5%)   | 1 (1%)   | 18          | 55  |
| 27  | N     | 127/130 (98%) | 123 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 28  | O     | 125/130 (96%) | 116 (93%) | 8 (6%)   | 1 (1%)   | 16          | 52  |
| 29  | P     | 97/103 (94%)  | 89 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 30  | Q     | 115/129 (89%) | 107 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 31  | R     | 117/124 (94%) | 112 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 32  | S     | 98/101 (97%)  | 97 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 33  | T     | 86/89 (97%)   | 83 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 34  | U     | 80/82 (98%)   | 76 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 35  | V     | 78/84 (93%)   | 74 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 36  | W     | 81/92 (88%)   | 80 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 37  | X     | 114/118 (97%) | 103 (90%) | 9 (8%)   | 2 (2%)   | 6           | 32  |
| 38  | Y     | 139/142 (98%) | 101 (73%) | 38 (27%) | 0        | 100         | 100 |
| 39  | Z     | 28/121 (23%)  | 22 (79%)  | 6 (21%)  | 0        | 100         | 100 |
| 41  | b     | 74/85 (87%)   | 73 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 42  | c     | 75/78 (96%)   | 72 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 44  | e     | 60/63 (95%)   | 57 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 45  | f     | 56/59 (95%)   | 52 (93%)  | 4 (7%)   | 0        | 100         | 100 |
| 46  | g     | 64/70 (91%)   | 62 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 47  | h     | 269/273 (98%) | 255 (95%) | 14 (5%)  | 0        | 100         | 100 |
| 48  | i     | 54/57 (95%)   | 49 (91%)  | 5 (9%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 49  | j     | 207/209 (99%)    | 198 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 50  | k     | 50/55 (91%)      | 50 (100%)  | 0        | 0        | 100         | 100 |
| 51  | l     | 199/201 (99%)    | 188 (94%)  | 11 (6%)  | 0        | 100         | 100 |
| 52  | m     | 44/46 (96%)      | 43 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 53  | n     | 175/179 (98%)    | 161 (92%)  | 13 (7%)  | 1 (1%)   | 21          | 58  |
| 54  | o     | 62/65 (95%)      | 57 (92%)   | 4 (6%)   | 1 (2%)   | 7           | 36  |
| 55  | p     | 173/177 (98%)    | 162 (94%)  | 11 (6%)  | 0        | 100         | 100 |
| 56  | q     | 36/38 (95%)      | 35 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 57  | r     | 147/149 (99%)    | 139 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 58  | s     | 140/142 (99%)    | 133 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 59  | t     | 121/123 (98%)    | 114 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 60  | u     | 142/144 (99%)    | 134 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 61  | v     | 134/136 (98%)    | 129 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 62  | w     | 117/127 (92%)    | 112 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 63  | x     | 114/117 (97%)    | 107 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 64  | y     | 112/115 (97%)    | 105 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 65  | z     | 115/118 (98%)    | 111 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| All | All   | 9486/10558 (90%) | 8740 (92%) | 713 (8%) | 33 (0%)  | 37          | 71  |

All (33) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | AB    | 141 | LEU  |
| 12  | AB    | 152 | HIS  |
| 20  | G     | 127 | ASP  |
| 21  | H     | 304 | VAL  |
| 26  | M     | 56  | LYS  |
| 54  | o     | 32  | ILE  |
| 14  | AE    | 92  | VAL  |
| 14  | AE    | 175 | GLU  |
| 21  | H     | 171 | ARG  |
| 21  | H     | 305 | HIS  |
| 21  | H     | 309 | MET  |
| 24  | K     | 78  | ASN  |
| 25  | L     | 96  | VAL  |
| 28  | O     | 13  | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | n     | 177  | PHE  |
| 12  | AB    | 160  | ARG  |
| 13  | AC    | 193  | GLU  |
| 21  | H     | 82   | THR  |
| 12  | AB    | 53   | ASN  |
| 14  | AE    | 74   | LYS  |
| 14  | AE    | 286  | ALA  |
| 21  | H     | 143  | ASP  |
| 37  | X     | 6    | GLY  |
| 37  | X     | 66   | GLU  |
| 9   | 9     | 79   | PRO  |
| 9   | 9     | 88   | HIS  |
| 12  | AB    | 137  | ALA  |
| 13  | AC    | 192  | VAL  |
| 14  | AE    | 290  | ILE  |
| 21  | H     | 71   | ALA  |
| 14  | AE    | 292  | VAL  |
| 9   | 9     | 129  | LEU  |
| 11  | AA    | 1317 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | 0     | 84/84 (100%)    | 84 (100%)   | 0        | 100         | 100 |
| 2   | 1     | 93/93 (100%)    | 93 (100%)   | 0        | 100         | 100 |
| 3   | 2     | 81/84 (96%)     | 81 (100%)   | 0        | 100         | 100 |
| 4   | 3     | 84/85 (99%)     | 84 (100%)   | 0        | 100         | 100 |
| 5   | 4     | 78/78 (100%)    | 78 (100%)   | 0        | 100         | 100 |
| 9   | 9     | 112/123 (91%)   | 112 (100%)  | 0        | 100         | 100 |
| 11  | AA    | 1135/1157 (98%) | 1130 (100%) | 5 (0%)   | 84          | 83  |
| 12  | AB    | 141/142 (99%)   | 139 (99%)   | 2 (1%)   | 59          | 71  |
| 13  | AC    | 186/286 (65%)   | 186 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 13  | AD    | 185/286 (65%)   | 185 (100%) | 0        | 100         | 100 |
| 14  | AE    | 1122/1168 (96%) | 1104 (98%) | 18 (2%)  | 55          | 69  |
| 15  | AF    | 70/75 (93%)     | 69 (99%)   | 1 (1%)   | 59          | 71  |
| 16  | C     | 57/65 (88%)     | 57 (100%)  | 0        | 100         | 100 |
| 18  | E     | 65/66 (98%)     | 65 (100%)  | 0        | 100         | 100 |
| 19  | F     | 60/61 (98%)     | 60 (100%)  | 0        | 100         | 100 |
| 20  | G     | 187/199 (94%)   | 187 (100%) | 0        | 100         | 100 |
| 21  | H     | 137/461 (30%)   | 137 (100%) | 0        | 100         | 100 |
| 22  | I     | 171/190 (90%)   | 171 (100%) | 0        | 100         | 100 |
| 23  | J     | 172/173 (99%)   | 171 (99%)  | 1 (1%)   | 78          | 81  |
| 24  | K     | 119/126 (94%)   | 119 (100%) | 0        | 100         | 100 |
| 25  | L     | 91/116 (78%)    | 91 (100%)  | 0        | 100         | 100 |
| 26  | M     | 124/147 (84%)   | 124 (100%) | 0        | 100         | 100 |
| 27  | N     | 104/105 (99%)   | 104 (100%) | 0        | 100         | 100 |
| 28  | O     | 105/107 (98%)   | 105 (100%) | 0        | 100         | 100 |
| 29  | P     | 86/90 (96%)     | 86 (100%)  | 0        | 100         | 100 |
| 30  | Q     | 90/99 (91%)     | 90 (100%)  | 0        | 100         | 100 |
| 31  | R     | 101/104 (97%)   | 101 (100%) | 0        | 100         | 100 |
| 32  | S     | 83/84 (99%)     | 83 (100%)  | 0        | 100         | 100 |
| 33  | T     | 76/77 (99%)     | 76 (100%)  | 0        | 100         | 100 |
| 34  | U     | 65/65 (100%)    | 65 (100%)  | 0        | 100         | 100 |
| 35  | V     | 74/78 (95%)     | 74 (100%)  | 0        | 100         | 100 |
| 36  | W     | 72/79 (91%)     | 72 (100%)  | 0        | 100         | 100 |
| 37  | X     | 94/96 (98%)     | 94 (100%)  | 0        | 100         | 100 |
| 38  | Y     | 109/110 (99%)   | 109 (100%) | 0        | 100         | 100 |
| 39  | Z     | 26/85 (31%)     | 26 (100%)  | 0        | 100         | 100 |
| 41  | b     | 58/63 (92%)     | 58 (100%)  | 0        | 100         | 100 |
| 42  | c     | 67/68 (98%)     | 67 (100%)  | 0        | 100         | 100 |
| 44  | e     | 54/55 (98%)     | 54 (100%)  | 0        | 100         | 100 |
| 45  | f     | 48/49 (98%)     | 48 (100%)  | 0        | 100         | 100 |
| 46  | g     | 59/62 (95%)     | 59 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 47  | h     | 216/218 (99%)   | 216 (100%)  | 0        | 100         | 100 |
| 48  | i     | 47/48 (98%)     | 47 (100%)   | 0        | 100         | 100 |
| 49  | j     | 164/164 (100%)  | 164 (100%)  | 0        | 100         | 100 |
| 50  | k     | 47/49 (96%)     | 47 (100%)   | 0        | 100         | 100 |
| 51  | l     | 165/165 (100%)  | 165 (100%)  | 0        | 100         | 100 |
| 52  | m     | 38/38 (100%)    | 38 (100%)   | 0        | 100         | 100 |
| 53  | n     | 148/150 (99%)   | 148 (100%)  | 0        | 100         | 100 |
| 54  | o     | 51/52 (98%)     | 51 (100%)   | 0        | 100         | 100 |
| 55  | p     | 136/138 (99%)   | 136 (100%)  | 0        | 100         | 100 |
| 56  | q     | 34/34 (100%)    | 34 (100%)   | 0        | 100         | 100 |
| 57  | r     | 114/114 (100%)  | 114 (100%)  | 0        | 100         | 100 |
| 58  | s     | 116/116 (100%)  | 116 (100%)  | 0        | 100         | 100 |
| 59  | t     | 104/104 (100%)  | 104 (100%)  | 0        | 100         | 100 |
| 60  | u     | 103/103 (100%)  | 103 (100%)  | 0        | 100         | 100 |
| 61  | v     | 109/109 (100%)  | 109 (100%)  | 0        | 100         | 100 |
| 62  | w     | 99/103 (96%)    | 99 (100%)   | 0        | 100         | 100 |
| 63  | x     | 86/87 (99%)     | 86 (100%)   | 0        | 100         | 100 |
| 64  | y     | 99/100 (99%)    | 99 (100%)   | 0        | 100         | 100 |
| 65  | z     | 89/90 (99%)     | 89 (100%)   | 0        | 100         | 100 |
| All | All   | 7890/8723 (90%) | 7863 (100%) | 27 (0%)  | 84          | 84  |

All (27) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | AA    | 145  | ILE  |
| 11  | AA    | 615  | VAL  |
| 11  | AA    | 914  | LYS  |
| 11  | AA    | 1076 | ILE  |
| 11  | AA    | 1151 | LEU  |
| 12  | AB    | 146  | ILE  |
| 12  | AB    | 148  | LYS  |
| 14  | AE    | 69   | GLU  |
| 14  | AE    | 70   | CYS  |
| 14  | AE    | 71   | LEU  |
| 14  | AE    | 74   | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 14  | AE    | 76   | LYS  |
| 14  | AE    | 77   | ARG  |
| 14  | AE    | 78   | LEU  |
| 14  | AE    | 79   | LYS  |
| 14  | AE    | 81   | ARG  |
| 14  | AE    | 84   | ILE  |
| 14  | AE    | 85   | CYS  |
| 14  | AE    | 92   | VAL  |
| 14  | AE    | 93   | THR  |
| 14  | AE    | 290  | ILE  |
| 14  | AE    | 291  | ILE  |
| 14  | AE    | 292  | VAL  |
| 14  | AE    | 514  | THR  |
| 14  | AE    | 1261 | LEU  |
| 15  | AF    | 63   | ILE  |
| 23  | J     | 47   | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 0     | 6    | GLN  |
| 1   | 0     | 82   | HIS  |
| 2   | 1     | 7    | HIS  |
| 2   | 1     | 9    | HIS  |
| 3   | 2     | 15   | HIS  |
| 9   | 9     | 9    | GLN  |
| 11  | AA    | 69   | GLN  |
| 11  | AA    | 314  | ASN  |
| 11  | AA    | 330  | HIS  |
| 11  | AA    | 343  | HIS  |
| 11  | AA    | 387  | ASN  |
| 11  | AA    | 513  | GLN  |
| 11  | AA    | 554  | HIS  |
| 11  | AA    | 580  | GLN  |
| 11  | AA    | 688  | GLN  |
| 11  | AA    | 808  | ASN  |
| 11  | AA    | 1237 | HIS  |
| 11  | AA    | 1268 | GLN  |
| 11  | AA    | 1288 | GLN  |
| 11  | AA    | 1299 | ASN  |
| 11  | AA    | 1313 | HIS  |
| 12  | AB    | 27   | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 12  | AB    | 65   | HIS  |
| 13  | AC    | 23   | HIS  |
| 13  | AD    | 66   | HIS  |
| 13  | AD    | 84   | ASN  |
| 13  | AD    | 117  | HIS  |
| 13  | AD    | 128  | HIS  |
| 13  | AD    | 227  | GLN  |
| 14  | AE    | 80   | HIS  |
| 14  | AE    | 157  | GLN  |
| 14  | AE    | 164  | GLN  |
| 14  | AE    | 232  | ASN  |
| 14  | AE    | 365  | GLN  |
| 14  | AE    | 424  | ASN  |
| 14  | AE    | 450  | HIS  |
| 14  | AE    | 469  | HIS  |
| 14  | AE    | 777  | HIS  |
| 14  | AE    | 910  | ASN  |
| 14  | AE    | 1108 | GLN  |
| 14  | AE    | 1197 | ASN  |
| 14  | AE    | 1235 | ASN  |
| 14  | AE    | 1238 | GLN  |
| 14  | AE    | 1326 | GLN  |
| 15  | AF    | 31   | GLN  |
| 15  | AF    | 62   | GLN  |
| 16  | C     | 54   | GLN  |
| 18  | E     | 13   | GLN  |
| 18  | E     | 61   | GLN  |
| 19  | F     | 9    | ASN  |
| 20  | G     | 18   | HIS  |
| 20  | G     | 39   | HIS  |
| 20  | G     | 94   | HIS  |
| 20  | G     | 109  | GLN  |
| 22  | I     | 3    | GLN  |
| 22  | I     | 6    | HIS  |
| 22  | I     | 8    | ASN  |
| 22  | I     | 32   | ASN  |
| 22  | I     | 190  | HIS  |
| 23  | J     | 36   | GLN  |
| 23  | J     | 131  | ASN  |
| 23  | J     | 198  | HIS  |
| 24  | K     | 89   | HIS  |
| 25  | L     | 3    | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | L     | 68  | GLN  |
| 26  | M     | 68  | ASN  |
| 26  | M     | 86  | GLN  |
| 28  | O     | 5   | GLN  |
| 28  | O     | 81  | HIS  |
| 28  | O     | 126 | GLN  |
| 29  | P     | 58  | ASN  |
| 31  | R     | 77  | HIS  |
| 32  | S     | 4   | GLN  |
| 33  | T     | 80  | GLN  |
| 34  | U     | 26  | ASN  |
| 34  | U     | 59  | HIS  |
| 38  | Y     | 5   | GLN  |
| 44  | e     | 25  | GLN  |
| 44  | e     | 31  | GLN  |
| 45  | f     | 20  | HIS  |
| 45  | f     | 49  | ASN  |
| 46  | g     | 33  | ASN  |
| 47  | h     | 53  | HIS  |
| 47  | h     | 90  | ASN  |
| 49  | j     | 173 | GLN  |
| 51  | l     | 92  | HIS  |
| 51  | l     | 156 | ASN  |
| 51  | l     | 163 | ASN  |
| 52  | m     | 29  | GLN  |
| 53  | n     | 5   | HIS  |
| 53  | n     | 81  | GLN  |
| 54  | o     | 24  | HIS  |
| 54  | o     | 28  | ASN  |
| 56  | q     | 13  | ASN  |
| 57  | r     | 133 | GLN  |
| 58  | s     | 132 | HIS  |
| 61  | v     | 13  | HIS  |
| 61  | v     | 45  | GLN  |
| 61  | v     | 97  | GLN  |
| 62  | w     | 18  | GLN  |
| 63  | x     | 19  | GLN  |
| 63  | x     | 29  | HIS  |
| 63  | x     | 38  | GLN  |
| 64  | y     | 10  | GLN  |
| 64  | y     | 77  | HIS  |
| 65  | z     | 37  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65  | z     | 72  | ASN  |
| 65  | z     | 81  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 10  | A     | 75/76 (98%)     | 29 (38%)          | 8 (10%)         |
| 10  | B     | 75/76 (98%)     | 29 (38%)          | 8 (10%)         |
| 17  | D     | 1514/1542 (98%) | 290 (19%)         | 20 (1%)         |
| 40  | a     | 2859/2904 (98%) | 511 (17%)         | 0               |
| 43  | d     | 119/120 (99%)   | 15 (12%)          | 0               |
| 8   | 7     | 37/38 (97%)     | 28 (75%)          | 5 (13%)         |
| All | All   | 4679/4756 (98%) | 902 (19%)         | 41 (0%)         |

All (902) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 7     | 3   | G    |
| 8   | 7     | 4   | U    |
| 8   | 7     | 5   | U    |
| 8   | 7     | 7   | U    |
| 8   | 7     | 8   | U    |
| 8   | 7     | 9   | U    |
| 8   | 7     | 10  | U    |
| 8   | 7     | 11  | U    |
| 8   | 7     | 12  | U    |
| 8   | 7     | 13  | U    |
| 8   | 7     | 14  | U    |
| 8   | 7     | 15  | U    |
| 8   | 7     | 16  | U    |
| 8   | 7     | 17  | U    |
| 8   | 7     | 18  | U    |
| 8   | 7     | 19  | U    |
| 8   | 7     | 20  | U    |
| 8   | 7     | 21  | U    |
| 8   | 7     | 22  | U    |
| 8   | 7     | 23  | U    |
| 8   | 7     | 24  | U    |
| 8   | 7     | 25  | G    |
| 8   | 7     | 26  | A    |
| 8   | 7     | 27  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 7     | 28  | U    |
| 8   | 7     | 29  | U    |
| 8   | 7     | 32  | U    |
| 8   | 7     | 34  | A    |
| 10  | A     | 2   | G    |
| 10  | A     | 6   | G    |
| 10  | A     | 7   | G    |
| 10  | A     | 8   | U    |
| 10  | A     | 10  | G    |
| 10  | A     | 13  | C    |
| 10  | A     | 14  | A    |
| 10  | A     | 16  | C    |
| 10  | A     | 17  | C    |
| 10  | A     | 18  | G    |
| 10  | A     | 19  | G    |
| 10  | A     | 20  | U    |
| 10  | A     | 21  | A    |
| 10  | A     | 22  | G    |
| 10  | A     | 23  | C    |
| 10  | A     | 30  | G    |
| 10  | A     | 46  | G    |
| 10  | A     | 47  | U    |
| 10  | A     | 48  | C    |
| 10  | A     | 49  | G    |
| 10  | A     | 52  | G    |
| 10  | A     | 57  | A    |
| 10  | A     | 58  | A    |
| 10  | A     | 59  | A    |
| 10  | A     | 61  | C    |
| 10  | A     | 66  | C    |
| 10  | A     | 69  | C    |
| 10  | A     | 71  | C    |
| 10  | A     | 73  | A    |
| 10  | B     | 2   | G    |
| 10  | B     | 6   | G    |
| 10  | B     | 7   | G    |
| 10  | B     | 8   | U    |
| 10  | B     | 10  | G    |
| 10  | B     | 13  | C    |
| 10  | B     | 14  | A    |
| 10  | B     | 16  | C    |
| 10  | B     | 17  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | B     | 18  | G    |
| 10  | B     | 19  | G    |
| 10  | B     | 20  | U    |
| 10  | B     | 21  | A    |
| 10  | B     | 22  | G    |
| 10  | B     | 23  | C    |
| 10  | B     | 30  | G    |
| 10  | B     | 46  | G    |
| 10  | B     | 47  | U    |
| 10  | B     | 48  | C    |
| 10  | B     | 49  | G    |
| 10  | B     | 52  | G    |
| 10  | B     | 57  | A    |
| 10  | B     | 58  | A    |
| 10  | B     | 59  | A    |
| 10  | B     | 61  | C    |
| 10  | B     | 66  | C    |
| 10  | B     | 69  | C    |
| 10  | B     | 71  | C    |
| 10  | B     | 73  | A    |
| 17  | D     | 4   | U    |
| 17  | D     | 5   | U    |
| 17  | D     | 9   | G    |
| 17  | D     | 22  | G    |
| 17  | D     | 29  | U    |
| 17  | D     | 32  | A    |
| 17  | D     | 39  | G    |
| 17  | D     | 47  | C    |
| 17  | D     | 48  | C    |
| 17  | D     | 50  | A    |
| 17  | D     | 51  | A    |
| 17  | D     | 52  | C    |
| 17  | D     | 54  | C    |
| 17  | D     | 68  | G    |
| 17  | D     | 69  | G    |
| 17  | D     | 71  | A    |
| 17  | D     | 72  | A    |
| 17  | D     | 74  | A    |
| 17  | D     | 76  | G    |
| 17  | D     | 82  | G    |
| 17  | D     | 83  | C    |
| 17  | D     | 84  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | D     | 87  | C    |
| 17  | D     | 90  | C    |
| 17  | D     | 94  | G    |
| 17  | D     | 95  | C    |
| 17  | D     | 96  | U    |
| 17  | D     | 108 | G    |
| 17  | D     | 120 | A    |
| 17  | D     | 121 | U    |
| 17  | D     | 122 | G    |
| 17  | D     | 131 | A    |
| 17  | D     | 141 | G    |
| 17  | D     | 144 | G    |
| 17  | D     | 148 | G    |
| 17  | D     | 149 | A    |
| 17  | D     | 160 | A    |
| 17  | D     | 164 | G    |
| 17  | D     | 173 | U    |
| 17  | D     | 181 | A    |
| 17  | D     | 182 | A    |
| 17  | D     | 183 | C    |
| 17  | D     | 184 | G    |
| 17  | D     | 197 | A    |
| 17  | D     | 198 | G    |
| 17  | D     | 204 | G    |
| 17  | D     | 208 | U    |
| 17  | D     | 209 | U    |
| 17  | D     | 210 | C    |
| 17  | D     | 211 | G    |
| 17  | D     | 212 | G    |
| 17  | D     | 216 | U    |
| 17  | D     | 226 | G    |
| 17  | D     | 245 | U    |
| 17  | D     | 247 | G    |
| 17  | D     | 251 | G    |
| 17  | D     | 253 | A    |
| 17  | D     | 258 | G    |
| 17  | D     | 262 | A    |
| 17  | D     | 266 | G    |
| 17  | D     | 267 | C    |
| 17  | D     | 271 | C    |
| 17  | D     | 279 | A    |
| 17  | D     | 289 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | D     | 299 | G    |
| 17  | D     | 306 | A    |
| 17  | D     | 321 | A    |
| 17  | D     | 328 | C    |
| 17  | D     | 329 | A    |
| 17  | D     | 332 | G    |
| 17  | D     | 347 | G    |
| 17  | D     | 352 | C    |
| 17  | D     | 353 | A    |
| 17  | D     | 354 | G    |
| 17  | D     | 355 | C    |
| 17  | D     | 367 | U    |
| 17  | D     | 372 | C    |
| 17  | D     | 373 | A    |
| 17  | D     | 376 | G    |
| 17  | D     | 382 | A    |
| 17  | D     | 384 | G    |
| 17  | D     | 392 | C    |
| 17  | D     | 397 | A    |
| 17  | D     | 398 | U    |
| 17  | D     | 406 | G    |
| 17  | D     | 411 | A    |
| 17  | D     | 412 | A    |
| 17  | D     | 413 | G    |
| 17  | D     | 414 | A    |
| 17  | D     | 421 | U    |
| 17  | D     | 422 | C    |
| 17  | D     | 424 | G    |
| 17  | D     | 429 | U    |
| 17  | D     | 446 | G    |
| 17  | D     | 451 | A    |
| 17  | D     | 457 | G    |
| 17  | D     | 458 | U    |
| 17  | D     | 463 | U    |
| 17  | D     | 464 | U    |
| 17  | D     | 467 | U    |
| 17  | D     | 468 | A    |
| 17  | D     | 469 | C    |
| 17  | D     | 478 | A    |
| 17  | D     | 479 | U    |
| 17  | D     | 481 | G    |
| 17  | D     | 484 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | D     | 485 | U    |
| 17  | D     | 486 | U    |
| 17  | D     | 496 | A    |
| 17  | D     | 497 | G    |
| 17  | D     | 505 | G    |
| 17  | D     | 511 | C    |
| 17  | D     | 518 | C    |
| 17  | D     | 519 | C    |
| 17  | D     | 526 | C    |
| 17  | D     | 531 | U    |
| 17  | D     | 532 | A    |
| 17  | D     | 533 | A    |
| 17  | D     | 542 | G    |
| 17  | D     | 547 | A    |
| 17  | D     | 559 | A    |
| 17  | D     | 564 | C    |
| 17  | D     | 568 | G    |
| 17  | D     | 572 | A    |
| 17  | D     | 573 | A    |
| 17  | D     | 576 | C    |
| 17  | D     | 577 | G    |
| 17  | D     | 579 | A    |
| 17  | D     | 596 | A    |
| 17  | D     | 628 | G    |
| 17  | D     | 633 | G    |
| 17  | D     | 649 | A    |
| 17  | D     | 650 | G    |
| 17  | D     | 653 | U    |
| 17  | D     | 665 | A    |
| 17  | D     | 695 | A    |
| 17  | D     | 700 | G    |
| 17  | D     | 723 | U    |
| 17  | D     | 724 | G    |
| 17  | D     | 731 | G    |
| 17  | D     | 734 | G    |
| 17  | D     | 735 | C    |
| 17  | D     | 747 | A    |
| 17  | D     | 748 | G    |
| 17  | D     | 755 | G    |
| 17  | D     | 760 | G    |
| 17  | D     | 777 | A    |
| 17  | D     | 793 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 17  | D     | 794  | A    |
| 17  | D     | 815  | A    |
| 17  | D     | 817  | C    |
| 17  | D     | 828  | U    |
| 17  | D     | 829  | G    |
| 17  | D     | 832  | G    |
| 17  | D     | 841  | C    |
| 17  | D     | 843  | U    |
| 17  | D     | 844  | G    |
| 17  | D     | 845  | A    |
| 17  | D     | 846  | G    |
| 17  | D     | 849  | G    |
| 17  | D     | 874  | G    |
| 17  | D     | 887  | G    |
| 17  | D     | 902  | G    |
| 17  | D     | 914  | A    |
| 17  | D     | 916  | U    |
| 17  | D     | 926  | G    |
| 17  | D     | 934  | C    |
| 17  | D     | 935  | A    |
| 17  | D     | 960  | U    |
| 17  | D     | 963  | G    |
| 17  | D     | 965  | U    |
| 17  | D     | 969  | A    |
| 17  | D     | 972  | C    |
| 17  | D     | 975  | A    |
| 17  | D     | 976  | G    |
| 17  | D     | 987  | G    |
| 17  | D     | 991  | U    |
| 17  | D     | 992  | U    |
| 17  | D     | 993  | G    |
| 17  | D     | 996  | A    |
| 17  | D     | 1004 | A    |
| 17  | D     | 1008 | U    |
| 17  | D     | 1009 | U    |
| 17  | D     | 1017 | U    |
| 17  | D     | 1018 | G    |
| 17  | D     | 1021 | A    |
| 17  | D     | 1024 | G    |
| 17  | D     | 1026 | G    |
| 17  | D     | 1028 | C    |
| 17  | D     | 1030 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 17  | D     | 1031 | C    |
| 17  | D     | 1037 | C    |
| 17  | D     | 1043 | G    |
| 17  | D     | 1044 | A    |
| 17  | D     | 1046 | A    |
| 17  | D     | 1065 | U    |
| 17  | D     | 1085 | U    |
| 17  | D     | 1094 | G    |
| 17  | D     | 1095 | U    |
| 17  | D     | 1099 | G    |
| 17  | D     | 1101 | A    |
| 17  | D     | 1108 | G    |
| 17  | D     | 1124 | G    |
| 17  | D     | 1133 | G    |
| 17  | D     | 1135 | U    |
| 17  | D     | 1136 | C    |
| 17  | D     | 1137 | C    |
| 17  | D     | 1139 | G    |
| 17  | D     | 1140 | C    |
| 17  | D     | 1141 | C    |
| 17  | D     | 1142 | G    |
| 17  | D     | 1143 | G    |
| 17  | D     | 1145 | A    |
| 17  | D     | 1146 | A    |
| 17  | D     | 1151 | A    |
| 17  | D     | 1152 | A    |
| 17  | D     | 1159 | U    |
| 17  | D     | 1167 | A    |
| 17  | D     | 1171 | A    |
| 17  | D     | 1174 | G    |
| 17  | D     | 1175 | G    |
| 17  | D     | 1176 | A    |
| 17  | D     | 1184 | G    |
| 17  | D     | 1193 | G    |
| 17  | D     | 1196 | A    |
| 17  | D     | 1197 | A    |
| 17  | D     | 1206 | G    |
| 17  | D     | 1211 | U    |
| 17  | D     | 1212 | U    |
| 17  | D     | 1213 | A    |
| 17  | D     | 1214 | C    |
| 17  | D     | 1215 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 17  | D     | 1226 | C    |
| 17  | D     | 1227 | A    |
| 17  | D     | 1228 | C    |
| 17  | D     | 1238 | A    |
| 17  | D     | 1257 | A    |
| 17  | D     | 1260 | G    |
| 17  | D     | 1275 | A    |
| 17  | D     | 1276 | G    |
| 17  | D     | 1278 | G    |
| 17  | D     | 1279 | G    |
| 17  | D     | 1280 | A    |
| 17  | D     | 1285 | A    |
| 17  | D     | 1286 | U    |
| 17  | D     | 1287 | A    |
| 17  | D     | 1299 | A    |
| 17  | D     | 1300 | G    |
| 17  | D     | 1302 | C    |
| 17  | D     | 1305 | G    |
| 17  | D     | 1312 | G    |
| 17  | D     | 1317 | C    |
| 17  | D     | 1320 | C    |
| 17  | D     | 1323 | G    |
| 17  | D     | 1338 | G    |
| 17  | D     | 1340 | A    |
| 17  | D     | 1346 | A    |
| 17  | D     | 1347 | G    |
| 17  | D     | 1353 | G    |
| 17  | D     | 1363 | A    |
| 17  | D     | 1370 | G    |
| 17  | D     | 1378 | C    |
| 17  | D     | 1379 | G    |
| 17  | D     | 1381 | U    |
| 17  | D     | 1391 | U    |
| 17  | D     | 1396 | A    |
| 17  | D     | 1397 | C    |
| 17  | D     | 1398 | A    |
| 17  | D     | 1404 | C    |
| 17  | D     | 1419 | G    |
| 17  | D     | 1429 | A    |
| 17  | D     | 1441 | A    |
| 17  | D     | 1446 | A    |
| 17  | D     | 1447 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 17  | D     | 1448 | C    |
| 17  | D     | 1452 | C    |
| 17  | D     | 1453 | G    |
| 17  | D     | 1475 | G    |
| 17  | D     | 1487 | G    |
| 17  | D     | 1491 | G    |
| 17  | D     | 1492 | A    |
| 17  | D     | 1493 | A    |
| 17  | D     | 1494 | G    |
| 17  | D     | 1497 | G    |
| 17  | D     | 1503 | A    |
| 17  | D     | 1506 | U    |
| 17  | D     | 1517 | G    |
| 17  | D     | 1529 | G    |
| 17  | D     | 1530 | G    |
| 17  | D     | 1534 | A    |
| 40  | a     | 4    | U    |
| 40  | a     | 10   | A    |
| 40  | a     | 15   | G    |
| 40  | a     | 23   | G    |
| 40  | a     | 34   | U    |
| 40  | a     | 35   | G    |
| 40  | a     | 46   | G    |
| 40  | a     | 58   | G    |
| 40  | a     | 60   | G    |
| 40  | a     | 62   | U    |
| 40  | a     | 63   | A    |
| 40  | a     | 71   | A    |
| 40  | a     | 74   | A    |
| 40  | a     | 75   | G    |
| 40  | a     | 83   | A    |
| 40  | a     | 84   | A    |
| 40  | a     | 85   | G    |
| 40  | a     | 96   | C    |
| 40  | a     | 101  | A    |
| 40  | a     | 102  | U    |
| 40  | a     | 103  | A    |
| 40  | a     | 110  | G    |
| 40  | a     | 118  | A    |
| 40  | a     | 119  | A    |
| 40  | a     | 120  | U    |
| 40  | a     | 131  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | a     | 136 | G    |
| 40  | a     | 139 | U    |
| 40  | a     | 140 | C    |
| 40  | a     | 141 | G    |
| 40  | a     | 163 | C    |
| 40  | a     | 165 | A    |
| 40  | a     | 181 | A    |
| 40  | a     | 196 | A    |
| 40  | a     | 215 | G    |
| 40  | a     | 216 | A    |
| 40  | a     | 222 | A    |
| 40  | a     | 225 | C    |
| 40  | a     | 248 | G    |
| 40  | a     | 249 | C    |
| 40  | a     | 261 | G    |
| 40  | a     | 264 | C    |
| 40  | a     | 265 | A    |
| 40  | a     | 266 | G    |
| 40  | a     | 267 | C    |
| 40  | a     | 271 | G    |
| 40  | a     | 272 | A    |
| 40  | a     | 275 | C    |
| 40  | a     | 276 | U    |
| 40  | a     | 278 | A    |
| 40  | a     | 285 | G    |
| 40  | a     | 291 | G    |
| 40  | a     | 311 | A    |
| 40  | a     | 329 | G    |
| 40  | a     | 330 | A    |
| 40  | a     | 353 | C    |
| 40  | a     | 361 | G    |
| 40  | a     | 362 | A    |
| 40  | a     | 371 | A    |
| 40  | a     | 372 | G    |
| 40  | a     | 373 | U    |
| 40  | a     | 375 | G    |
| 40  | a     | 383 | C    |
| 40  | a     | 386 | G    |
| 40  | a     | 396 | G    |
| 40  | a     | 405 | U    |
| 40  | a     | 411 | G    |
| 40  | a     | 412 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | a     | 420 | C    |
| 40  | a     | 424 | G    |
| 40  | a     | 451 | U    |
| 40  | a     | 457 | A    |
| 40  | a     | 477 | A    |
| 40  | a     | 481 | G    |
| 40  | a     | 491 | G    |
| 40  | a     | 501 | A    |
| 40  | a     | 503 | A    |
| 40  | a     | 504 | A    |
| 40  | a     | 505 | A    |
| 40  | a     | 509 | C    |
| 40  | a     | 522 | A    |
| 40  | a     | 529 | A    |
| 40  | a     | 531 | C    |
| 40  | a     | 532 | A    |
| 40  | a     | 537 | G    |
| 40  | a     | 543 | G    |
| 40  | a     | 545 | U    |
| 40  | a     | 546 | U    |
| 40  | a     | 547 | A    |
| 40  | a     | 549 | G    |
| 40  | a     | 551 | G    |
| 40  | a     | 563 | A    |
| 40  | a     | 569 | U    |
| 40  | a     | 573 | U    |
| 40  | a     | 575 | A    |
| 40  | a     | 588 | U    |
| 40  | a     | 603 | A    |
| 40  | a     | 609 | A    |
| 40  | a     | 613 | A    |
| 40  | a     | 614 | A    |
| 40  | a     | 615 | U    |
| 40  | a     | 616 | A    |
| 40  | a     | 627 | A    |
| 40  | a     | 637 | A    |
| 40  | a     | 645 | C    |
| 40  | a     | 647 | G    |
| 40  | a     | 654 | A    |
| 40  | a     | 668 | A    |
| 40  | a     | 686 | U    |
| 40  | a     | 710 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | a     | 717 | C    |
| 40  | a     | 730 | A    |
| 40  | a     | 738 | G    |
| 40  | a     | 757 | G    |
| 40  | a     | 764 | A    |
| 40  | a     | 765 | C    |
| 40  | a     | 775 | G    |
| 40  | a     | 776 | G    |
| 40  | a     | 782 | A    |
| 40  | a     | 784 | G    |
| 40  | a     | 785 | G    |
| 40  | a     | 800 | A    |
| 40  | a     | 805 | G    |
| 40  | a     | 812 | C    |
| 40  | a     | 819 | A    |
| 40  | a     | 827 | U    |
| 40  | a     | 828 | U    |
| 40  | a     | 845 | A    |
| 40  | a     | 846 | U    |
| 40  | a     | 858 | G    |
| 40  | a     | 859 | G    |
| 40  | a     | 869 | G    |
| 40  | a     | 878 | A    |
| 40  | a     | 881 | G    |
| 40  | a     | 884 | U    |
| 40  | a     | 885 | C    |
| 40  | a     | 888 | C    |
| 40  | a     | 891 | G    |
| 40  | a     | 895 | U    |
| 40  | a     | 896 | A    |
| 40  | a     | 897 | C    |
| 40  | a     | 899 | A    |
| 40  | a     | 907 | G    |
| 40  | a     | 910 | A    |
| 40  | a     | 914 | G    |
| 40  | a     | 915 | C    |
| 40  | a     | 931 | U    |
| 40  | a     | 941 | A    |
| 40  | a     | 945 | A    |
| 40  | a     | 946 | C    |
| 40  | a     | 953 | G    |
| 40  | a     | 961 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 974  | G    |
| 40  | a     | 983  | A    |
| 40  | a     | 995  | C    |
| 40  | a     | 996  | A    |
| 40  | a     | 999  | U    |
| 40  | a     | 1005 | C    |
| 40  | a     | 1012 | U    |
| 40  | a     | 1013 | C    |
| 40  | a     | 1022 | G    |
| 40  | a     | 1023 | U    |
| 40  | a     | 1026 | G    |
| 40  | a     | 1033 | U    |
| 40  | a     | 1041 | G    |
| 40  | a     | 1045 | C    |
| 40  | a     | 1046 | A    |
| 40  | a     | 1047 | G    |
| 40  | a     | 1060 | U    |
| 40  | a     | 1061 | U    |
| 40  | a     | 1064 | C    |
| 40  | a     | 1065 | U    |
| 40  | a     | 1066 | U    |
| 40  | a     | 1067 | A    |
| 40  | a     | 1068 | G    |
| 40  | a     | 1070 | A    |
| 40  | a     | 1071 | G    |
| 40  | a     | 1073 | A    |
| 40  | a     | 1074 | G    |
| 40  | a     | 1079 | C    |
| 40  | a     | 1080 | A    |
| 40  | a     | 1081 | U    |
| 40  | a     | 1082 | U    |
| 40  | a     | 1083 | U    |
| 40  | a     | 1084 | A    |
| 40  | a     | 1087 | G    |
| 40  | a     | 1088 | A    |
| 40  | a     | 1090 | A    |
| 40  | a     | 1095 | A    |
| 40  | a     | 1101 | U    |
| 40  | a     | 1107 | G    |
| 40  | a     | 1110 | G    |
| 40  | a     | 1111 | A    |
| 40  | a     | 1112 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 1119 | U    |
| 40  | a     | 1122 | G    |
| 40  | a     | 1128 | G    |
| 40  | a     | 1132 | U    |
| 40  | a     | 1134 | A    |
| 40  | a     | 1135 | C    |
| 40  | a     | 1142 | A    |
| 40  | a     | 1169 | A    |
| 40  | a     | 1170 | C    |
| 40  | a     | 1173 | U    |
| 40  | a     | 1174 | U    |
| 40  | a     | 1175 | A    |
| 40  | a     | 1176 | U    |
| 40  | a     | 1177 | G    |
| 40  | a     | 1178 | C    |
| 40  | a     | 1179 | G    |
| 40  | a     | 1180 | U    |
| 40  | a     | 1186 | G    |
| 40  | a     | 1238 | G    |
| 40  | a     | 1248 | G    |
| 40  | a     | 1253 | A    |
| 40  | a     | 1256 | G    |
| 40  | a     | 1266 | G    |
| 40  | a     | 1271 | G    |
| 40  | a     | 1272 | A    |
| 40  | a     | 1273 | U    |
| 40  | a     | 1300 | G    |
| 40  | a     | 1301 | A    |
| 40  | a     | 1321 | A    |
| 40  | a     | 1345 | C    |
| 40  | a     | 1352 | U    |
| 40  | a     | 1365 | A    |
| 40  | a     | 1368 | G    |
| 40  | a     | 1378 | A    |
| 40  | a     | 1379 | U    |
| 40  | a     | 1380 | G    |
| 40  | a     | 1383 | A    |
| 40  | a     | 1392 | A    |
| 40  | a     | 1395 | A    |
| 40  | a     | 1406 | U    |
| 40  | a     | 1408 | G    |
| 40  | a     | 1409 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 1414 | C    |
| 40  | a     | 1416 | G    |
| 40  | a     | 1417 | C    |
| 40  | a     | 1419 | A    |
| 40  | a     | 1420 | A    |
| 40  | a     | 1428 | C    |
| 40  | a     | 1452 | G    |
| 40  | a     | 1453 | A    |
| 40  | a     | 1460 | U    |
| 40  | a     | 1482 | G    |
| 40  | a     | 1490 | A    |
| 40  | a     | 1497 | U    |
| 40  | a     | 1503 | A    |
| 40  | a     | 1508 | A    |
| 40  | a     | 1509 | A    |
| 40  | a     | 1510 | G    |
| 40  | a     | 1515 | A    |
| 40  | a     | 1529 | G    |
| 40  | a     | 1534 | U    |
| 40  | a     | 1535 | A    |
| 40  | a     | 1536 | C    |
| 40  | a     | 1537 | G    |
| 40  | a     | 1554 | U    |
| 40  | a     | 1559 | U    |
| 40  | a     | 1566 | A    |
| 40  | a     | 1569 | A    |
| 40  | a     | 1578 | U    |
| 40  | a     | 1580 | A    |
| 40  | a     | 1581 | G    |
| 40  | a     | 1582 | C    |
| 40  | a     | 1583 | A    |
| 40  | a     | 1584 | U    |
| 40  | a     | 1585 | C    |
| 40  | a     | 1589 | U    |
| 40  | a     | 1590 | A    |
| 40  | a     | 1608 | A    |
| 40  | a     | 1610 | A    |
| 40  | a     | 1613 | G    |
| 40  | a     | 1647 | U    |
| 40  | a     | 1648 | U    |
| 40  | a     | 1649 | G    |
| 40  | a     | 1651 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 1665 | A    |
| 40  | a     | 1674 | G    |
| 40  | a     | 1677 | A    |
| 40  | a     | 1703 | G    |
| 40  | a     | 1714 | U    |
| 40  | a     | 1715 | G    |
| 40  | a     | 1729 | U    |
| 40  | a     | 1730 | C    |
| 40  | a     | 1732 | C    |
| 40  | a     | 1738 | G    |
| 40  | a     | 1750 | G    |
| 40  | a     | 1758 | U    |
| 40  | a     | 1764 | C    |
| 40  | a     | 1773 | A    |
| 40  | a     | 1791 | A    |
| 40  | a     | 1800 | C    |
| 40  | a     | 1808 | A    |
| 40  | a     | 1811 | G    |
| 40  | a     | 1816 | C    |
| 40  | a     | 1829 | A    |
| 40  | a     | 1833 | C    |
| 40  | a     | 1847 | A    |
| 40  | a     | 1848 | A    |
| 40  | a     | 1858 | A    |
| 40  | a     | 1859 | U    |
| 40  | a     | 1862 | G    |
| 40  | a     | 1864 | U    |
| 40  | a     | 1869 | G    |
| 40  | a     | 1870 | C    |
| 40  | a     | 1872 | A    |
| 40  | a     | 1873 | G    |
| 40  | a     | 1906 | G    |
| 40  | a     | 1907 | G    |
| 40  | a     | 1913 | A    |
| 40  | a     | 1914 | C    |
| 40  | a     | 1919 | A    |
| 40  | a     | 1920 | C    |
| 40  | a     | 1922 | G    |
| 40  | a     | 1923 | U    |
| 40  | a     | 1924 | C    |
| 40  | a     | 1925 | C    |
| 40  | a     | 1926 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 1929 | G    |
| 40  | a     | 1930 | G    |
| 40  | a     | 1936 | A    |
| 40  | a     | 1938 | A    |
| 40  | a     | 1955 | U    |
| 40  | a     | 1965 | C    |
| 40  | a     | 1967 | C    |
| 40  | a     | 1970 | A    |
| 40  | a     | 1971 | U    |
| 40  | a     | 1972 | G    |
| 40  | a     | 1987 | A    |
| 40  | a     | 1991 | U    |
| 40  | a     | 1992 | G    |
| 40  | a     | 1993 | U    |
| 40  | a     | 1997 | C    |
| 40  | a     | 2002 | G    |
| 40  | a     | 2020 | A    |
| 40  | a     | 2022 | U    |
| 40  | a     | 2023 | C    |
| 40  | a     | 2027 | G    |
| 40  | a     | 2033 | A    |
| 40  | a     | 2043 | C    |
| 40  | a     | 2051 | A    |
| 40  | a     | 2052 | A    |
| 40  | a     | 2055 | C    |
| 40  | a     | 2056 | G    |
| 40  | a     | 2060 | A    |
| 40  | a     | 2061 | G    |
| 40  | a     | 2062 | A    |
| 40  | a     | 2063 | C    |
| 40  | a     | 2097 | A    |
| 40  | a     | 2099 | U    |
| 40  | a     | 2100 | G    |
| 40  | a     | 2108 | A    |
| 40  | a     | 2110 | G    |
| 40  | a     | 2111 | U    |
| 40  | a     | 2113 | U    |
| 40  | a     | 2115 | G    |
| 40  | a     | 2116 | G    |
| 40  | a     | 2117 | A    |
| 40  | a     | 2118 | U    |
| 40  | a     | 2121 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 2122 | U    |
| 40  | a     | 2124 | G    |
| 40  | a     | 2125 | G    |
| 40  | a     | 2126 | A    |
| 40  | a     | 2127 | G    |
| 40  | a     | 2128 | G    |
| 40  | a     | 2131 | U    |
| 40  | a     | 2132 | U    |
| 40  | a     | 2133 | G    |
| 40  | a     | 2134 | A    |
| 40  | a     | 2139 | U    |
| 40  | a     | 2141 | G    |
| 40  | a     | 2146 | C    |
| 40  | a     | 2147 | A    |
| 40  | a     | 2154 | A    |
| 40  | a     | 2157 | G    |
| 40  | a     | 2158 | A    |
| 40  | a     | 2159 | G    |
| 40  | a     | 2162 | G    |
| 40  | a     | 2163 | A    |
| 40  | a     | 2164 | C    |
| 40  | a     | 2165 | C    |
| 40  | a     | 2169 | A    |
| 40  | a     | 2171 | A    |
| 40  | a     | 2172 | U    |
| 40  | a     | 2178 | C    |
| 40  | a     | 2182 | U    |
| 40  | a     | 2183 | A    |
| 40  | a     | 2185 | U    |
| 40  | a     | 2189 | U    |
| 40  | a     | 2190 | G    |
| 40  | a     | 2193 | G    |
| 40  | a     | 2194 | U    |
| 40  | a     | 2198 | A    |
| 40  | a     | 2204 | G    |
| 40  | a     | 2211 | A    |
| 40  | a     | 2212 | A    |
| 40  | a     | 2225 | A    |
| 40  | a     | 2226 | C    |
| 40  | a     | 2229 | U    |
| 40  | a     | 2238 | G    |
| 40  | a     | 2239 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 2250 | G    |
| 40  | a     | 2268 | A    |
| 40  | a     | 2278 | A    |
| 40  | a     | 2283 | C    |
| 40  | a     | 2287 | A    |
| 40  | a     | 2288 | A    |
| 40  | a     | 2297 | A    |
| 40  | a     | 2305 | U    |
| 40  | a     | 2308 | G    |
| 40  | a     | 2309 | A    |
| 40  | a     | 2322 | A    |
| 40  | a     | 2325 | G    |
| 40  | a     | 2327 | A    |
| 40  | a     | 2333 | A    |
| 40  | a     | 2335 | A    |
| 40  | a     | 2339 | C    |
| 40  | a     | 2345 | G    |
| 40  | a     | 2347 | C    |
| 40  | a     | 2350 | C    |
| 40  | a     | 2361 | G    |
| 40  | a     | 2372 | U    |
| 40  | a     | 2376 | A    |
| 40  | a     | 2383 | G    |
| 40  | a     | 2385 | C    |
| 40  | a     | 2402 | U    |
| 40  | a     | 2403 | C    |
| 40  | a     | 2406 | A    |
| 40  | a     | 2423 | U    |
| 40  | a     | 2424 | C    |
| 40  | a     | 2425 | A    |
| 40  | a     | 2426 | A    |
| 40  | a     | 2429 | G    |
| 40  | a     | 2430 | A    |
| 40  | a     | 2431 | U    |
| 40  | a     | 2434 | A    |
| 40  | a     | 2435 | A    |
| 40  | a     | 2441 | U    |
| 40  | a     | 2447 | G    |
| 40  | a     | 2448 | A    |
| 40  | a     | 2470 | G    |
| 40  | a     | 2474 | U    |
| 40  | a     | 2476 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 2478 | A    |
| 40  | a     | 2484 | G    |
| 40  | a     | 2491 | U    |
| 40  | a     | 2502 | G    |
| 40  | a     | 2506 | U    |
| 40  | a     | 2512 | C    |
| 40  | a     | 2513 | A    |
| 40  | a     | 2518 | A    |
| 40  | a     | 2520 | C    |
| 40  | a     | 2525 | G    |
| 40  | a     | 2529 | G    |
| 40  | a     | 2535 | G    |
| 40  | a     | 2554 | U    |
| 40  | a     | 2566 | A    |
| 40  | a     | 2567 | G    |
| 40  | a     | 2573 | C    |
| 40  | a     | 2574 | G    |
| 40  | a     | 2585 | U    |
| 40  | a     | 2586 | U    |
| 40  | a     | 2602 | A    |
| 40  | a     | 2603 | G    |
| 40  | a     | 2609 | U    |
| 40  | a     | 2610 | C    |
| 40  | a     | 2611 | C    |
| 40  | a     | 2613 | U    |
| 40  | a     | 2629 | U    |
| 40  | a     | 2630 | G    |
| 40  | a     | 2663 | G    |
| 40  | a     | 2669 | G    |
| 40  | a     | 2671 | G    |
| 40  | a     | 2689 | U    |
| 40  | a     | 2690 | U    |
| 40  | a     | 2714 | G    |
| 40  | a     | 2716 | C    |
| 40  | a     | 2726 | A    |
| 40  | a     | 2744 | G    |
| 40  | a     | 2748 | A    |
| 40  | a     | 2758 | A    |
| 40  | a     | 2765 | A    |
| 40  | a     | 2777 | G    |
| 40  | a     | 2778 | A    |
| 40  | a     | 2791 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 2793 | C    |
| 40  | a     | 2796 | U    |
| 40  | a     | 2797 | U    |
| 40  | a     | 2798 | U    |
| 40  | a     | 2799 | A    |
| 40  | a     | 2801 | G    |
| 40  | a     | 2818 | U    |
| 40  | a     | 2820 | A    |
| 40  | a     | 2823 | A    |
| 40  | a     | 2825 | G    |
| 40  | a     | 2835 | A    |
| 40  | a     | 2849 | U    |
| 40  | a     | 2859 | G    |
| 40  | a     | 2861 | U    |
| 40  | a     | 2867 | G    |
| 40  | a     | 2873 | A    |
| 40  | a     | 2874 | C    |
| 40  | a     | 2880 | C    |
| 40  | a     | 2883 | A    |
| 40  | a     | 2884 | U    |
| 40  | a     | 2885 | G    |
| 40  | a     | 2891 | U    |
| 40  | a     | 2902 | C    |
| 43  | d     | 2    | G    |
| 43  | d     | 13   | G    |
| 43  | d     | 16   | G    |
| 43  | d     | 17   | C    |
| 43  | d     | 35   | C    |
| 43  | d     | 45   | A    |
| 43  | d     | 51   | G    |
| 43  | d     | 56   | G    |
| 43  | d     | 57   | A    |
| 43  | d     | 66   | A    |
| 43  | d     | 88   | C    |
| 43  | d     | 89   | U    |
| 43  | d     | 90   | C    |
| 43  | d     | 99   | A    |
| 43  | d     | 109  | A    |

All (41) RNA pucker outliers are listed below:

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

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 7     | 4    | U    |
| 8   | 7     | 7    | U    |
| 8   | 7     | 10   | U    |
| 8   | 7     | 18   | U    |
| 8   | 7     | 24   | U    |
| 10  | A     | 6    | G    |
| 10  | A     | 7    | G    |
| 10  | A     | 9    | G    |
| 10  | A     | 12   | G    |
| 10  | A     | 21   | A    |
| 10  | A     | 22   | G    |
| 10  | A     | 57   | A    |
| 10  | A     | 60   | U    |
| 10  | B     | 6    | G    |
| 10  | B     | 7    | G    |
| 10  | B     | 9    | G    |
| 10  | B     | 12   | G    |
| 10  | B     | 21   | A    |
| 10  | B     | 22   | G    |
| 10  | B     | 57   | A    |
| 10  | B     | 60   | U    |
| 17  | D     | 121  | U    |
| 17  | D     | 181  | A    |
| 17  | D     | 183  | C    |
| 17  | D     | 197  | A    |
| 17  | D     | 209  | U    |
| 17  | D     | 428  | G    |
| 17  | D     | 496  | A    |
| 17  | D     | 517  | G    |
| 17  | D     | 991  | U    |
| 17  | D     | 992  | U    |
| 17  | D     | 1145 | A    |
| 17  | D     | 1196 | A    |
| 17  | D     | 1211 | U    |
| 17  | D     | 1212 | U    |
| 17  | D     | 1213 | A    |
| 17  | D     | 1214 | C    |
| 17  | D     | 1447 | A    |
| 17  | D     | 1491 | G    |
| 17  | D     | 1492 | A    |
| 17  | D     | 1493 | A    |

## 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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.

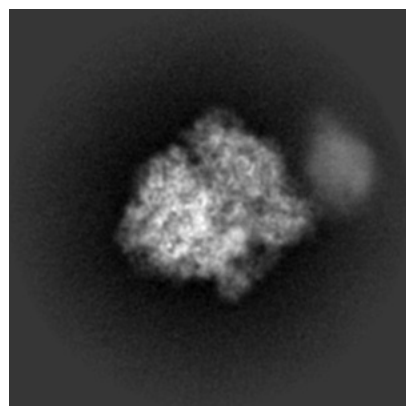
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42454. These allow visual inspection of the internal detail of the map and identification of artifacts.

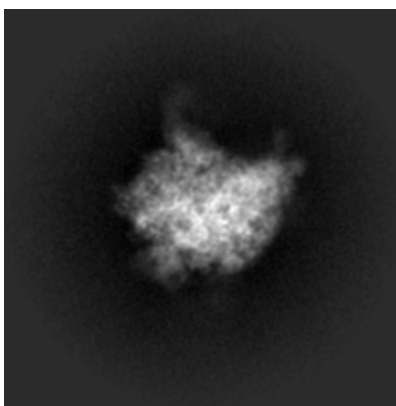
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

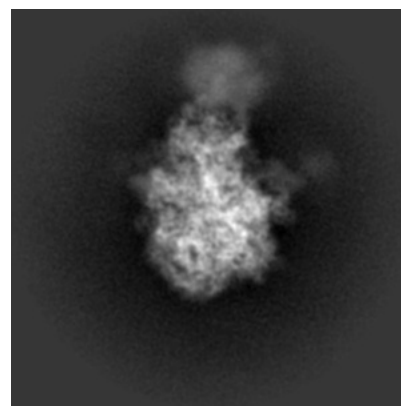
#### 6.1.1 Primary map



X

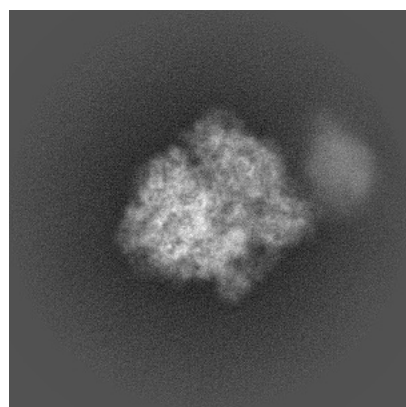


Y

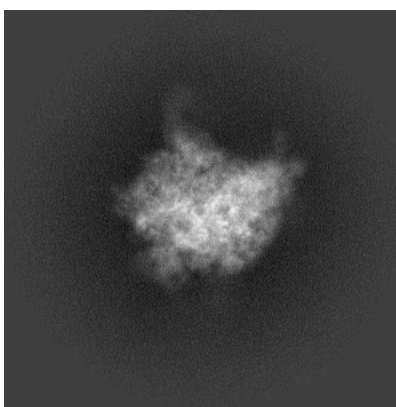


Z

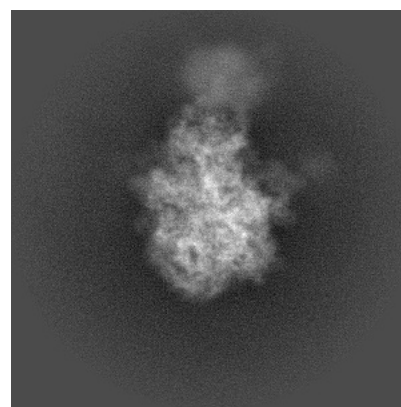
#### 6.1.2 Raw map



X



Y

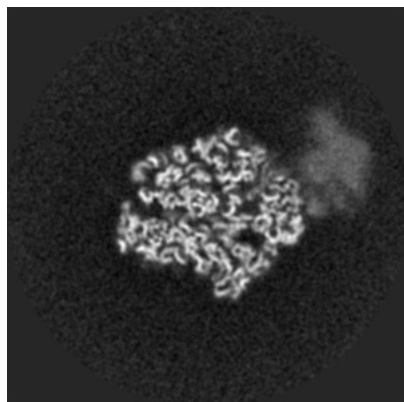


Z

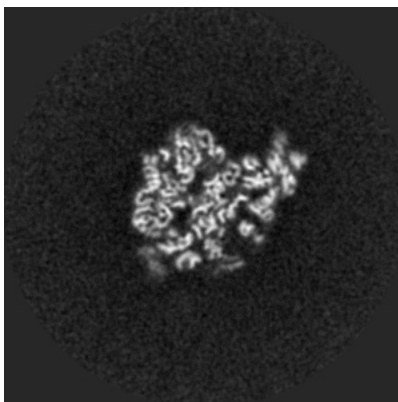
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

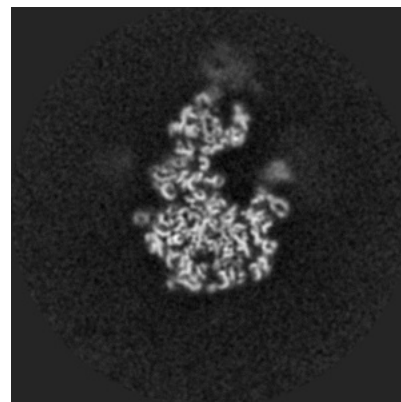
### 6.2.1 Primary map



X Index: 256

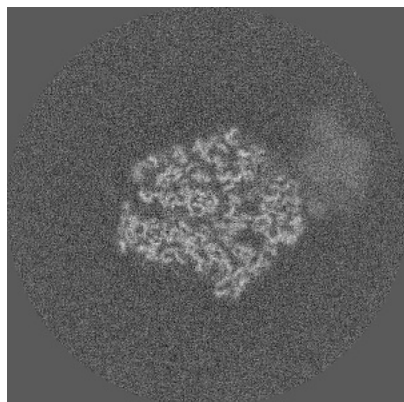


Y Index: 256

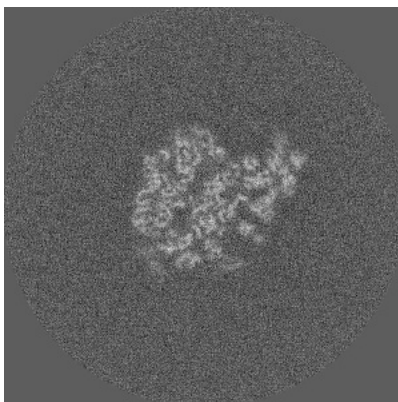


Z Index: 256

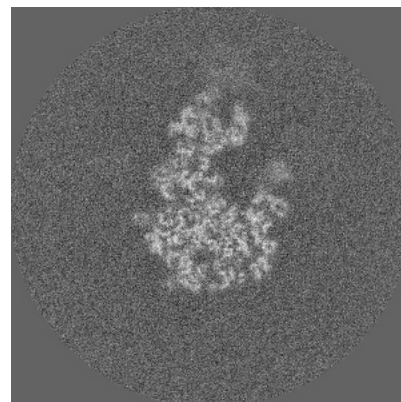
### 6.2.2 Raw map



X Index: 256



Y Index: 256

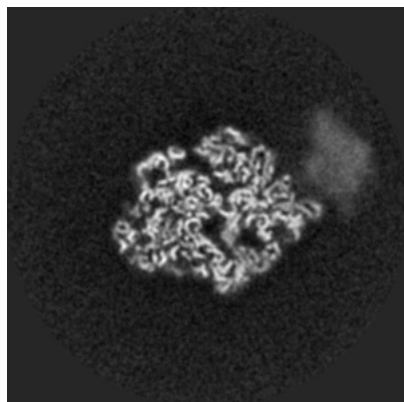


Z Index: 256

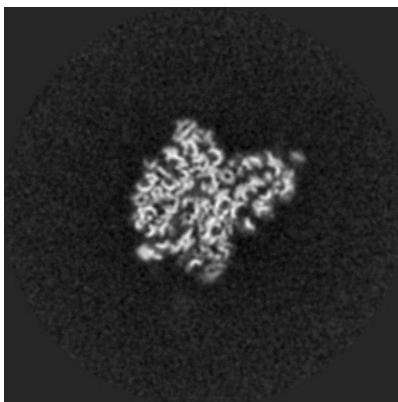
The images above show central slices of the map in three orthogonal directions.

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

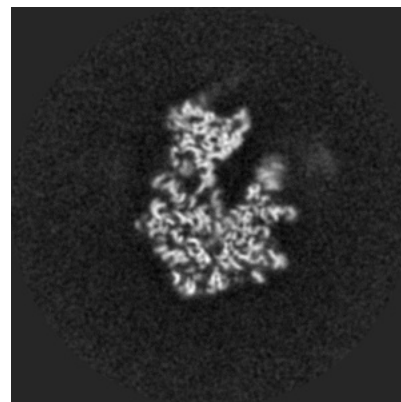
### 6.3.1 Primary map



X Index: 248

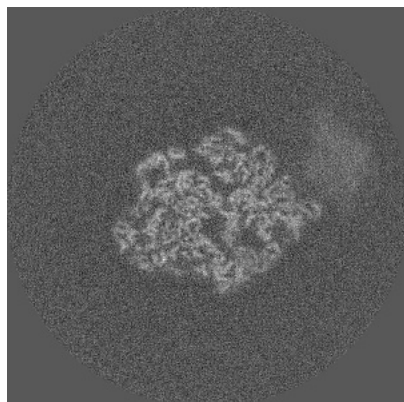


Y Index: 249

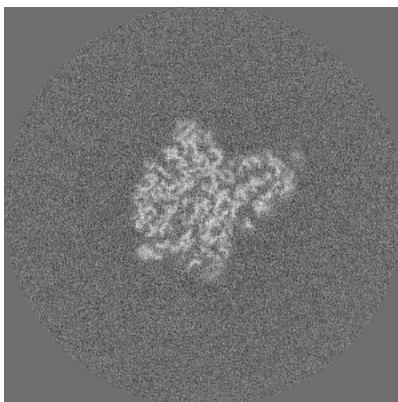


Z Index: 241

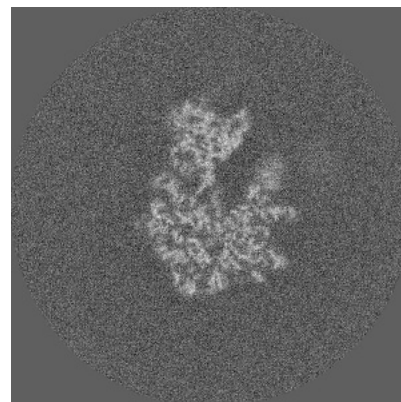
### 6.3.2 Raw map



X Index: 248



Y Index: 249



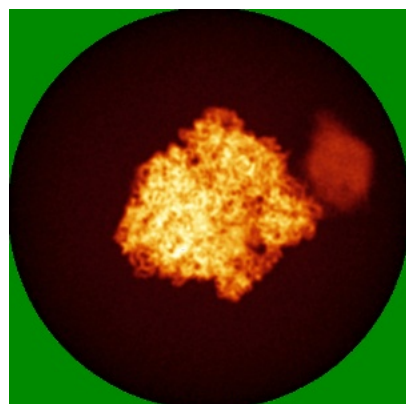
Z Index: 241

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



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

### 6.4.1 Primary map



X

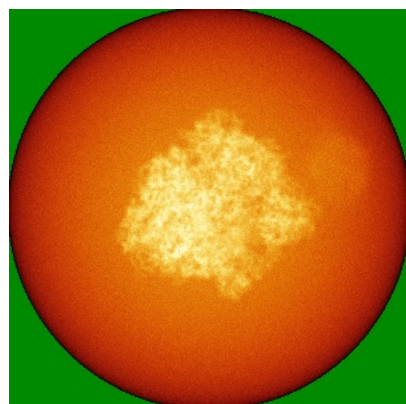


Y

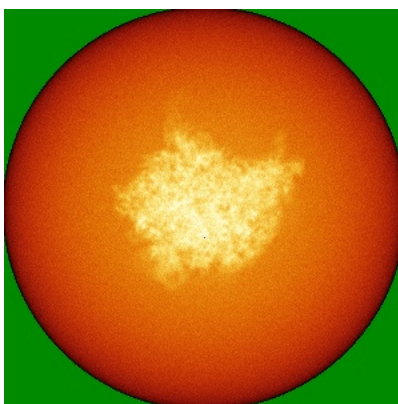


Z

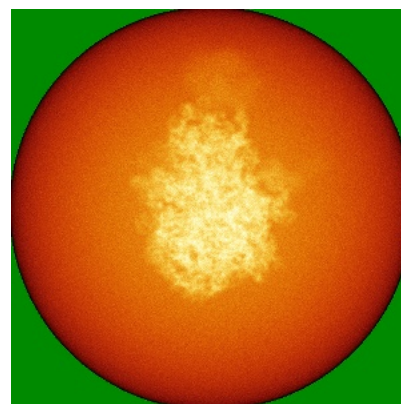
### 6.4.2 Raw map



X



Y

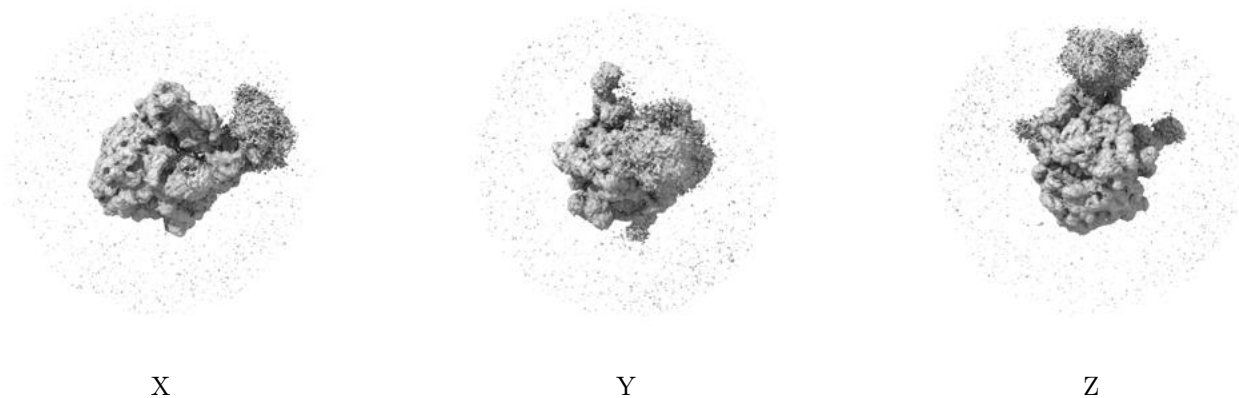


Z

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

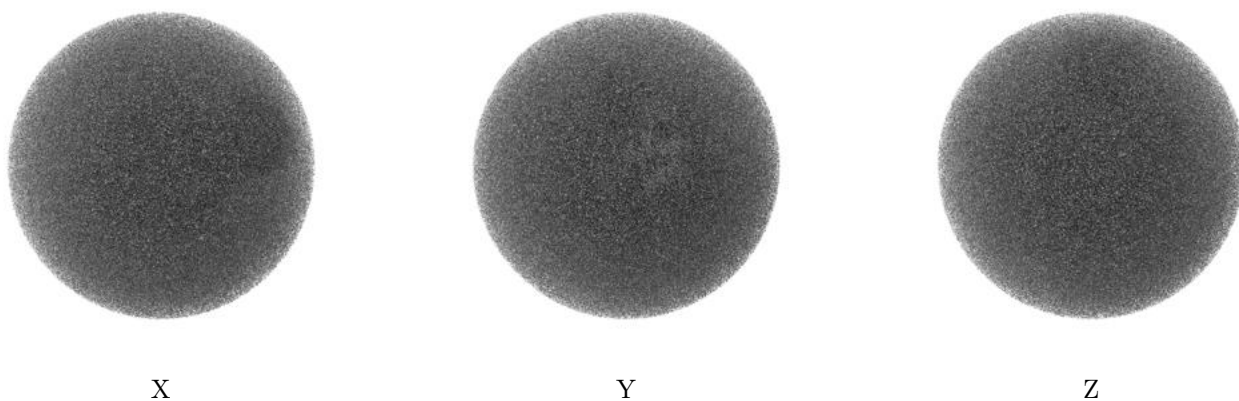
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

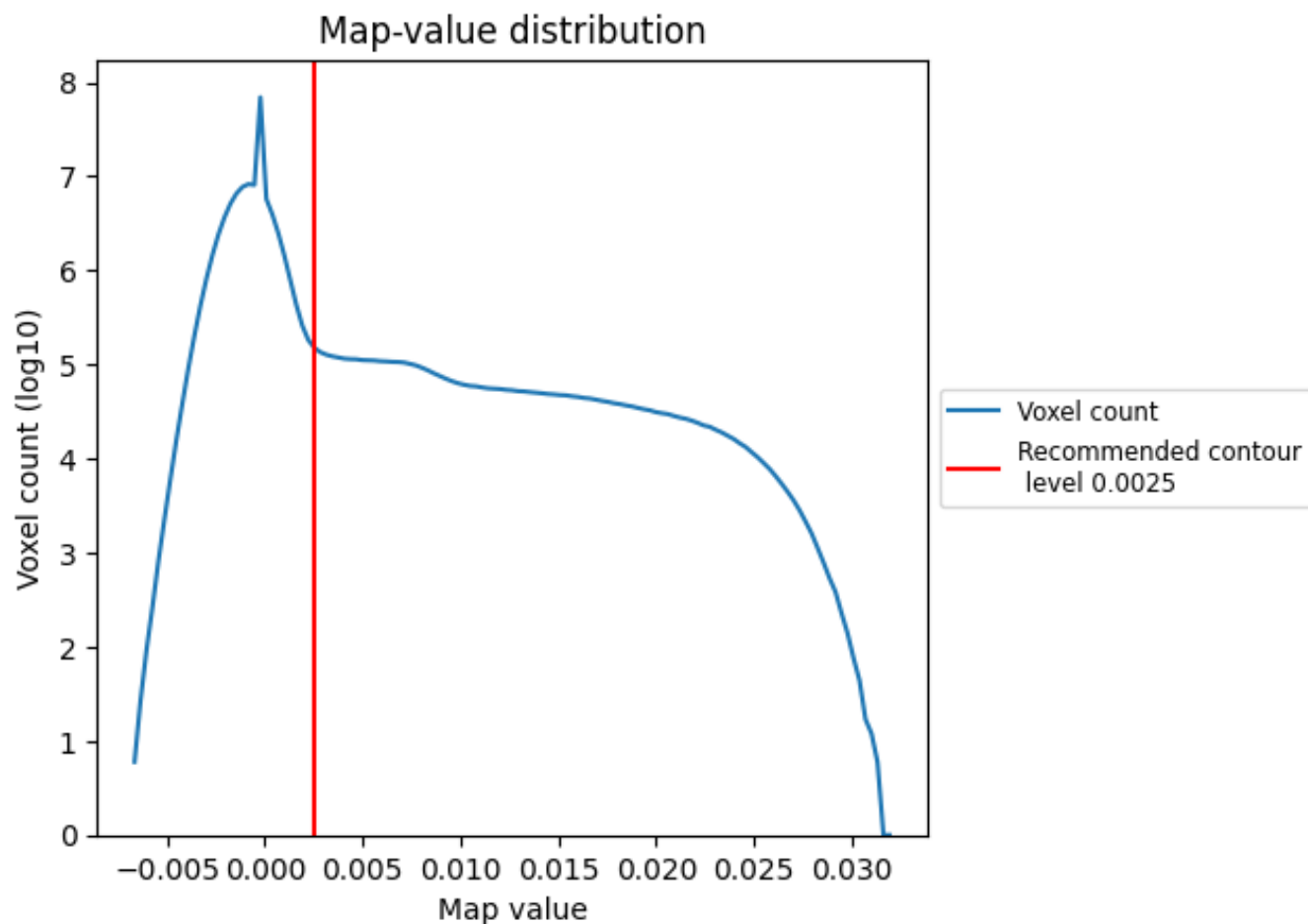
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

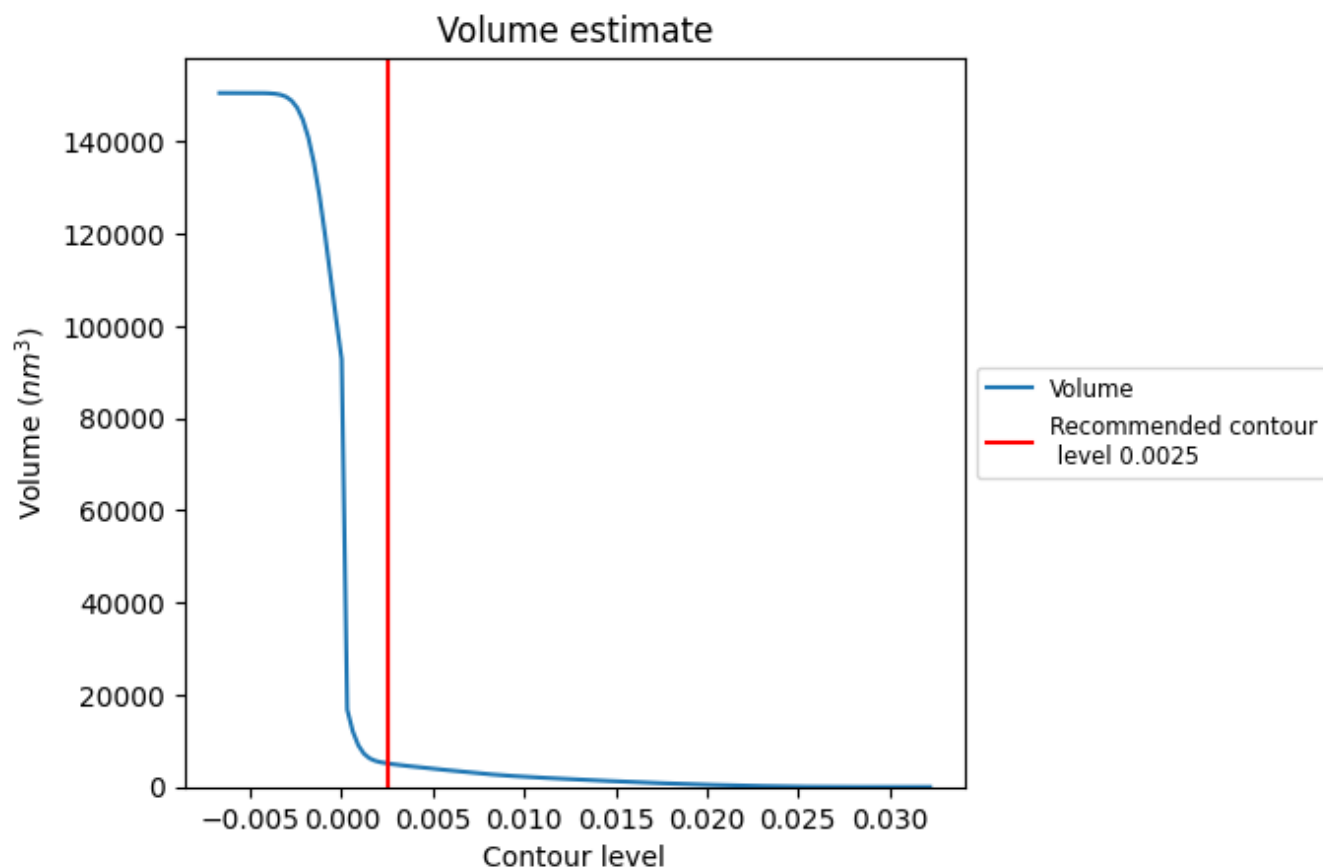
### 7.1 Map-value distribution [i](#)



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



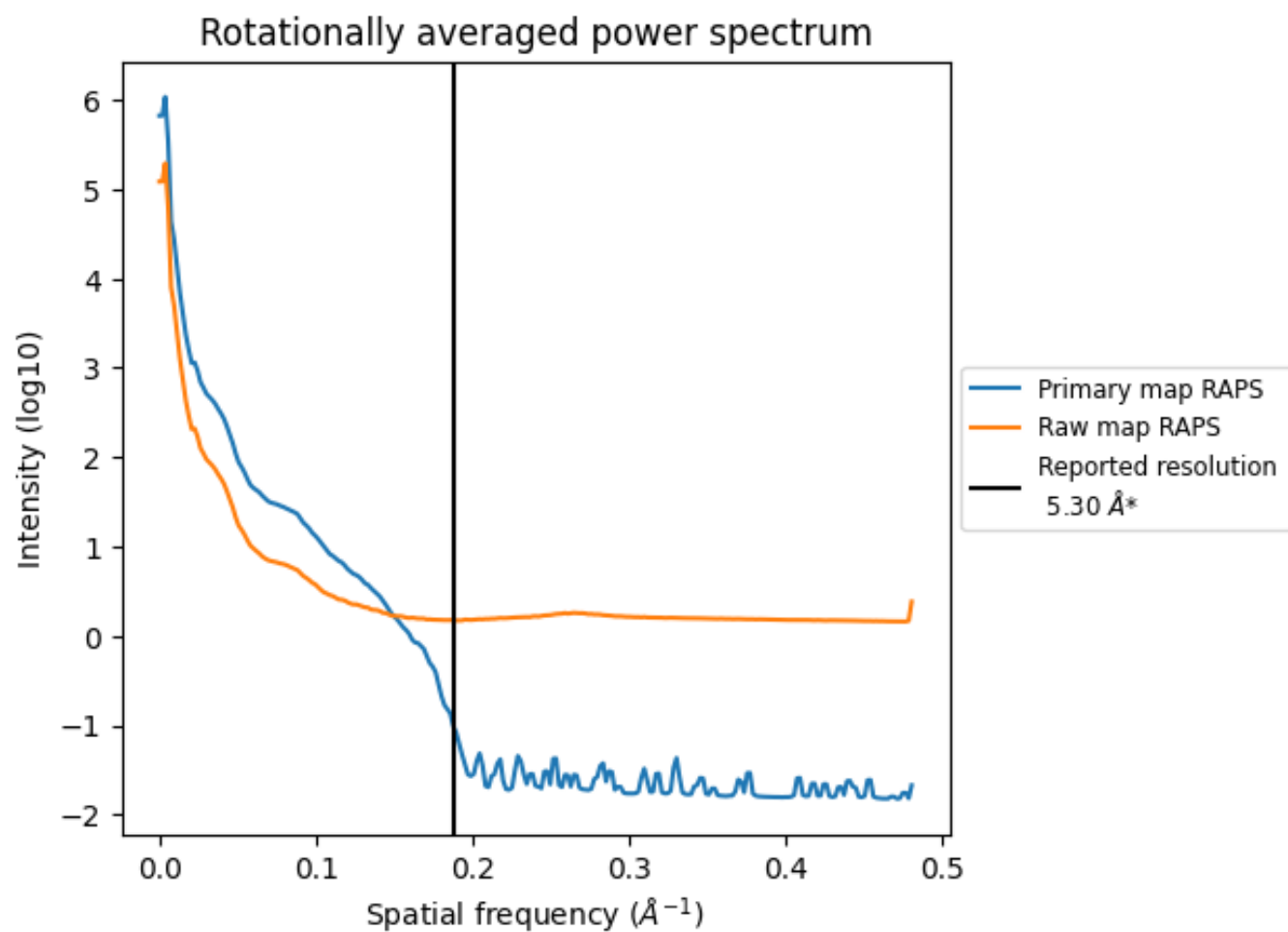
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5120 nm<sup>3</sup>; this corresponds to an approximate mass of 4625 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 ⓘ

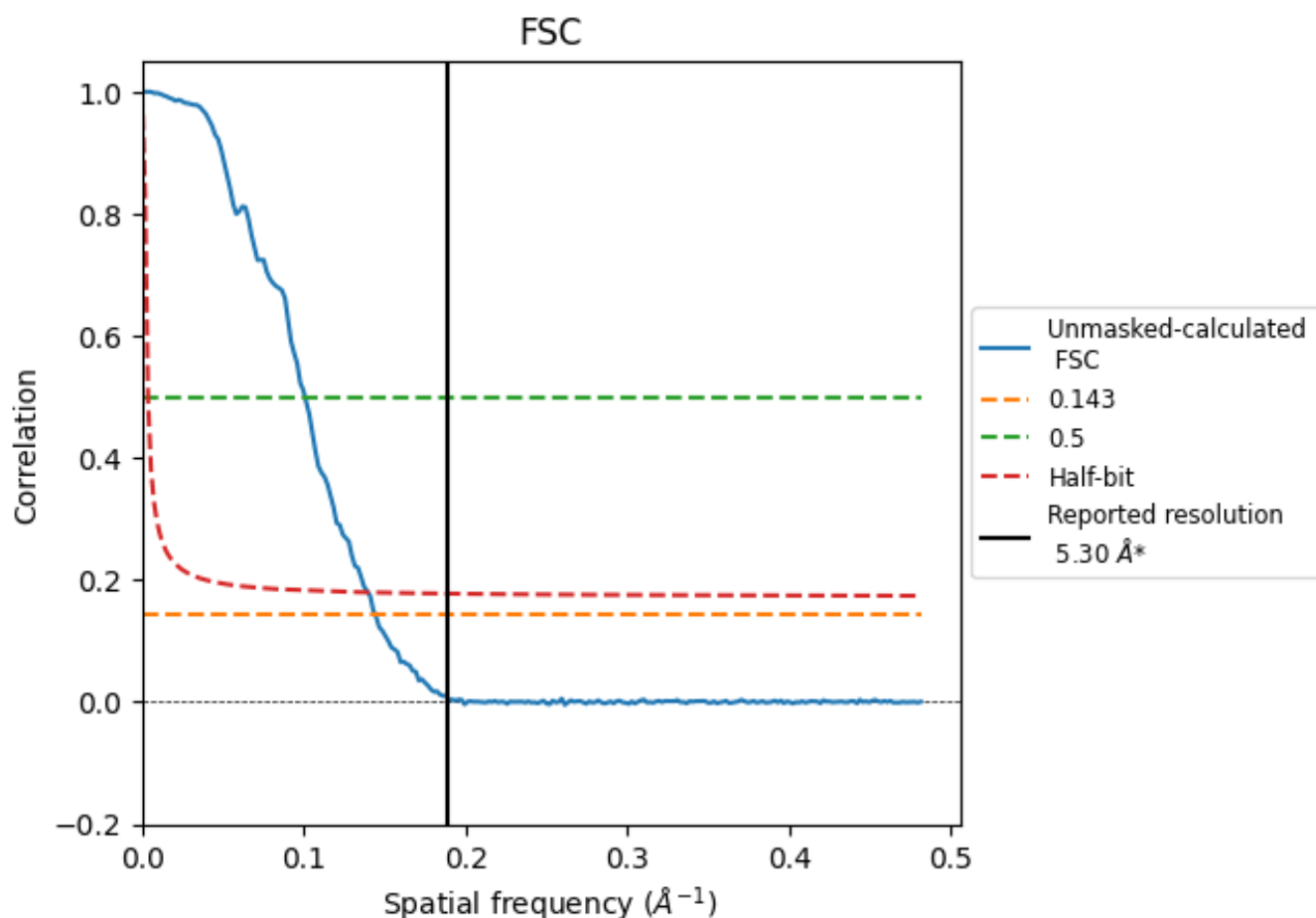


\*Reported resolution corresponds to spatial frequency of 0.189 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.189 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

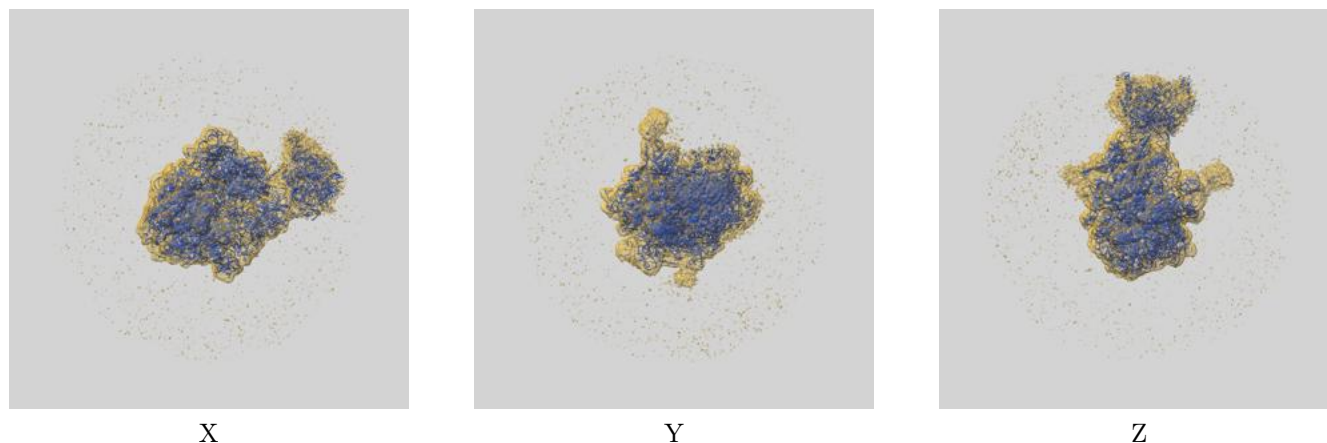
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 5.30                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 6.94                               | 9.93 | 7.16     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.94 differs from the reported value 5.3 by more than 10 %

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

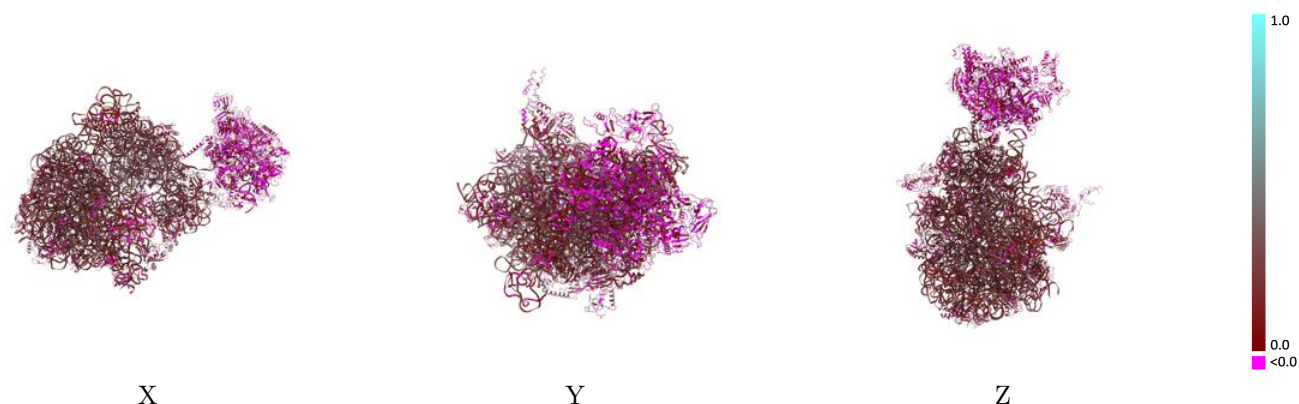
This section contains information regarding the fit between EMDB map EMD-42454 and PDB model 8UPR. Per-residue inclusion information can be found in section 3 on page 16.

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



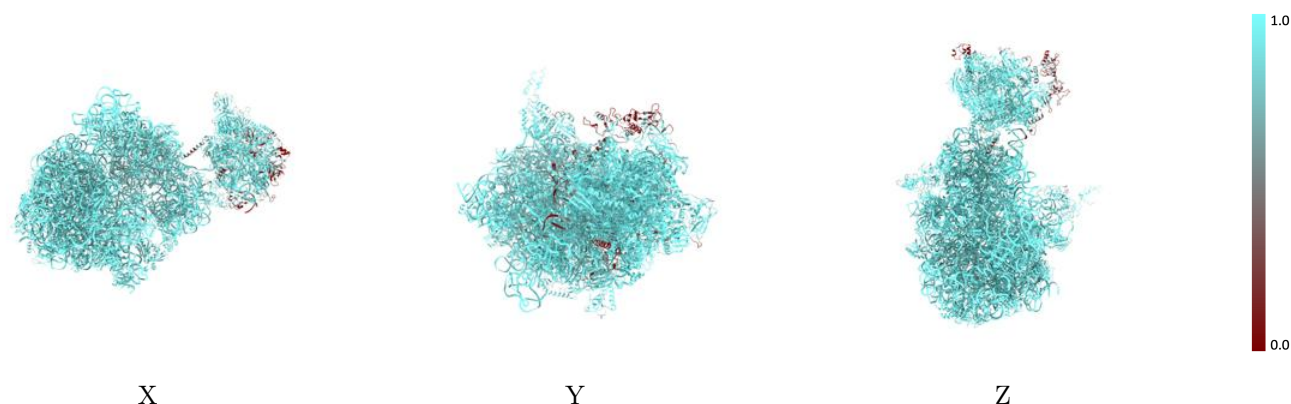
The images above show the 3D surface view of the map at the recommended contour level 0.0025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



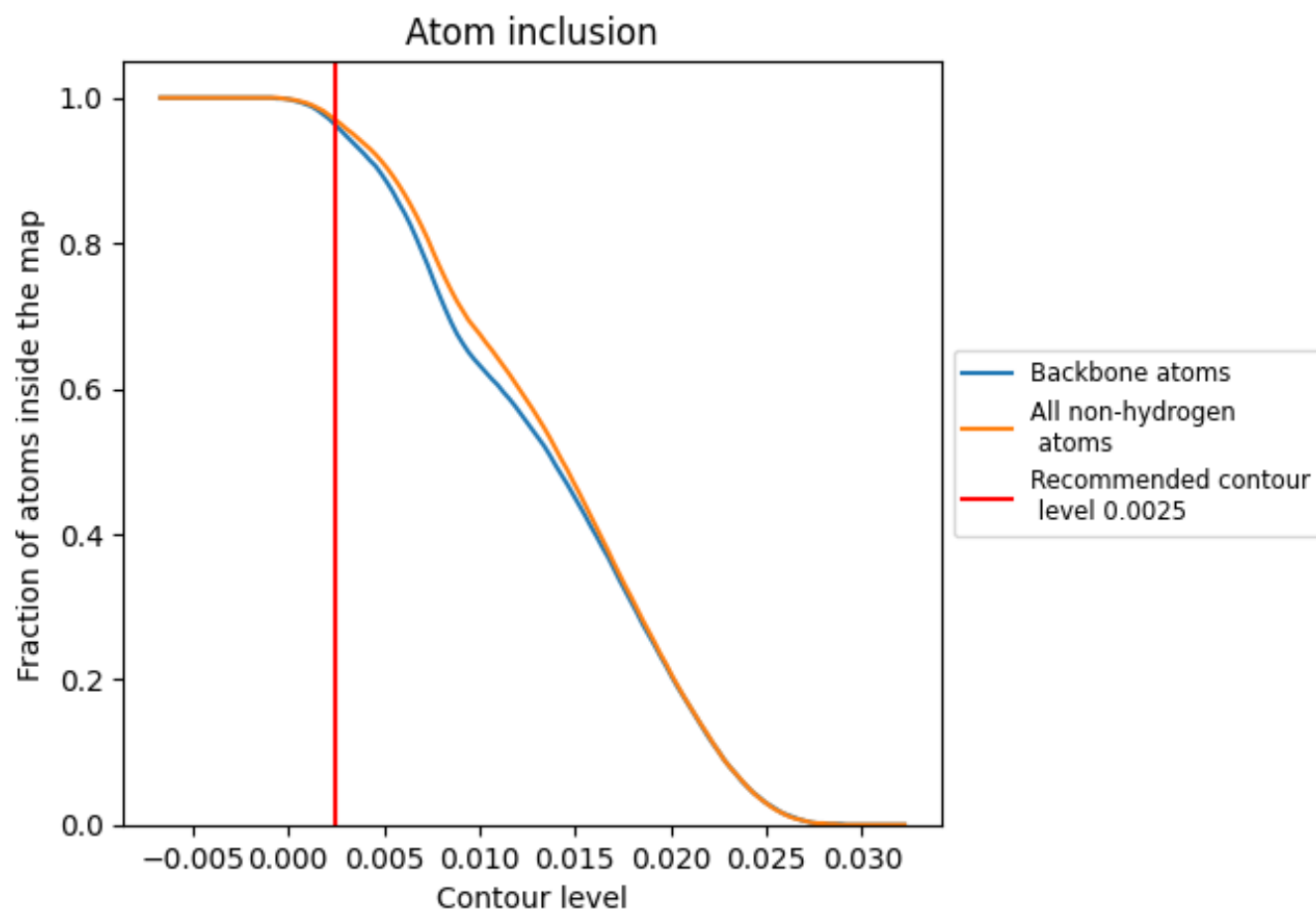
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0025).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 97% 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 (0.0025) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9690   |  0.1640   |
| 0     |  0.9940   |  0.1470   |
| 1     |  0.9960   |  0.1770   |
| 2     |  0.9840   |  0.1390   |
| 3     |  0.9960   |  0.1320   |
| 4     |  0.9950   |  0.1550   |
| 5     |  0.8440   |  0.0630   |
| 6     |  0.8950   |  0.0530   |
| 7     |  0.9820   |  0.0800   |
| 9     |  0.9740   |  0.0970   |
| A     |  1.0000   |  0.1790   |
| AA    |  0.8530   |  0.0180   |
| AB    |  0.7320   |  0.0520   |
| AC    |  0.9780   |  0.0280   |
| AD    |  0.9450  |  0.0160  |
| AE    |  0.8920 |  0.0320 |
| AF    |  0.7900 |  0.0190 |
| B     |  0.9800 |  0.1100 |
| C     |  0.9980 |  0.1530 |
| D     |  0.9980 |  0.2210 |
| E     |  0.9990 |  0.1540 |
| F     |  0.9820 |  0.1740 |
| G     |  0.9850 |  0.1580 |
| H     |  0.9140 |  0.0630 |
| I     |  0.9920 |  0.1870 |
| J     |  0.9980 |  0.1730 |
| K     |  0.9970 |  0.2020 |
| L     |  1.0000 |  0.1540 |
| M     |  0.9930 |  0.1490 |
| N     |  0.9870 |  0.1750 |
| O     |  0.9910 |  0.1280 |
| P     |  1.0000 |  0.1580 |
| Q     |  0.9970 |  0.1510 |
| R     |  0.9980 |  0.2050 |
| S     |  0.9970 |  0.1650 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| T     |  1.0000   |  0.1490   |
| U     |  0.9980   |  0.1610   |
| V     |  0.9910   |  0.1670   |
| W     |  0.9750   |  0.1230   |
| X     |  0.9930   |  0.1390   |
| Y     |  0.9010   |  0.0550   |
| Z     |  0.9690   |  0.0340   |
| a     |  0.9990   |  0.2090   |
| b     |  0.9970   |  0.1270   |
| c     |  0.9920   |  0.1580   |
| d     |  1.0000   |  0.1810   |
| e     |  0.9920   |  0.1320   |
| f     |  0.9930   |  0.1740   |
| g     |  0.9940   |  0.1140   |
| h     |  0.9930   |  0.1500   |
| i     |  0.9910   |  0.1870   |
| j     |  0.9960   |  0.1550   |
| k     |  1.0000   |  0.1360   |
| l     |  0.9890   |  0.1340   |
| m     |  0.9940  |  0.1680  |
| n     |  0.9880 |  0.1240 |
| o     |  1.0000 |  0.1240 |
| p     |  0.9980 |  0.1480 |
| q     |  0.9970 |  0.1410 |
| r     |  0.9660 |  0.1120 |
| s     |  0.9960 |  0.1710 |
| t     |  0.9900 |  0.1740 |
| u     |  0.9940 |  0.1280 |
| v     |  0.9920 |  0.1800 |
| w     |  0.9950 |  0.1510 |
| x     |  0.9820 |  0.0900 |
| y     |  0.9940 |  0.1690 |
| z     |  0.9970 |  0.1390 |