



## Full wwPDB EM Validation Report ⓘ

Jun 30, 2026 – 01:16 PM JST

PDB ID : 9UZK / pdb\_00009uzk  
EMDB ID : EMD-64644  
Title : EMCV IRES captured on mammalian 40S with initiator tRNA  
Authors : Das, D.; Hussain, T.  
Deposited on : 2025-05-16  
Resolution : 4.60 Å (reported)  
Based on initial models : ., 6YAN, 8OZ0

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.dev133  
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) : 2.50

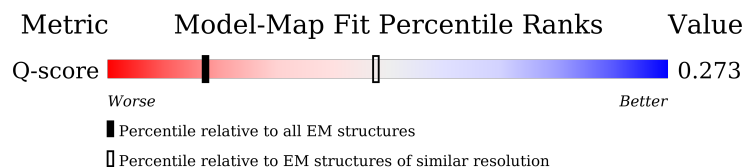
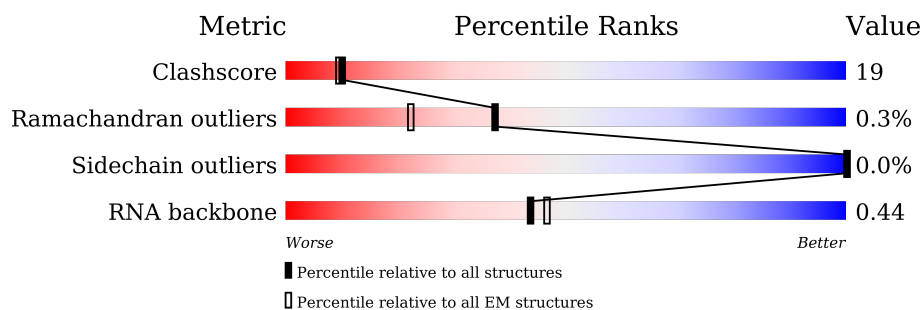
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.60 Å.

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



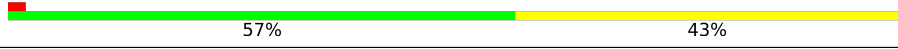
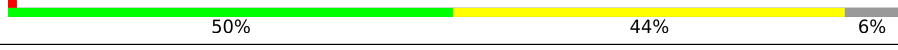
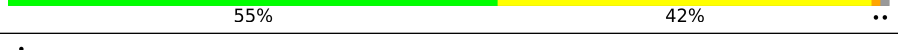
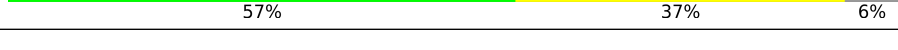
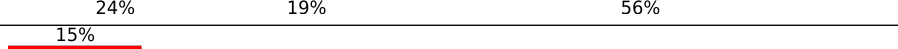
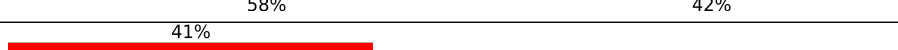
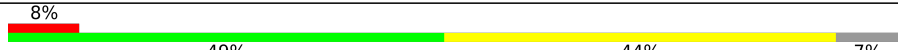
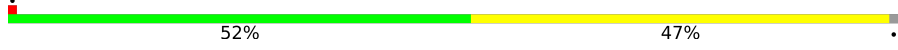
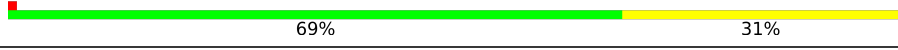
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 2407 ( 4.10 - 5.10 )                                     |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 2     | 1863   |                  |
| 2   | C     | 295    |                  |
| 3   | D     | 264    |                  |

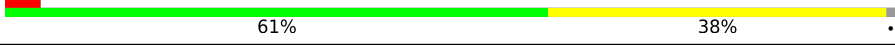
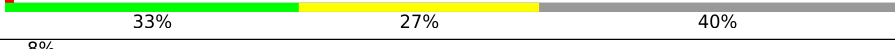
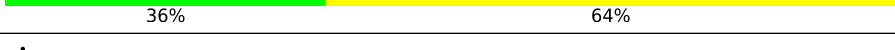
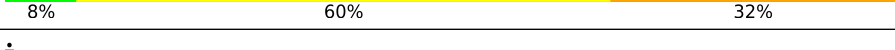
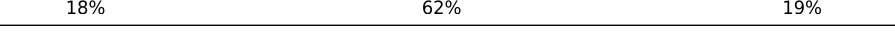
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | E     | 226    |    |
| 5   | F     | 243    |    |
| 6   | G     | 263    |    |
| 7   | H     | 204    |    |
| 8   | I     | 249    |    |
| 9   | J     | 194    |    |
| 10  | K     | 208    |    |
| 11  | L     | 194    |    |
| 12  | M     | 225    |    |
| 13  | N     | 158    |    |
| 14  | O     | 132    |    |
| 15  | P     | 151    |  |
| 16  | Q     | 168    |  |
| 17  | R     | 145    |  |
| 18  | S     | 146    |  |
| 19  | T     | 135    |  |
| 20  | U     | 152    |  |
| 21  | V     | 141    |  |
| 22  | W     | 119    |  |
| 23  | X     | 83     |  |
| 24  | Y     | 130    |  |
| 25  | Z     | 143    |  |
| 26  | a     | 126    |  |
| 27  | b     | 115    |  |
| 28  | c     | 84     |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 29  | d     | 64     |  |
| 30  | e     | 56     |  |
| 31  | f     | 156    |  |
| 32  | g     | 317    |  |
| 33  | h     | 125    |  |
| 34  | i     | 59     |  |
| 35  | l     | 25     |  |
| 36  | y     | 75     |  |
| 37  | z     | 93     |  |

## 2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 80043 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | 2     | 1744     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 37194 | 16608 | 6662 | 12184 | 1740 |         |       |

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | C     | 208      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1642  | 1045 | 289 | 300 | 8 |         |       |

- Molecule 3 is a protein called Small ribosomal subunit protein eS1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | D     | 215      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1741  | 1107 | 309 | 310 | 15 |         |       |

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | E     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1721  | 1114 | 295 | 303 | 9 |         |       |

- Molecule 5 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | F     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1764  | 1124 | 317 | 315 | 8 |         |       |

- Molecule 6 is a protein called Small ribosomal subunit protein eS4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | G     | 263      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2083  | 1329 | 385 | 359 | 10 |         |       |

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | H     | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1509  | 943 | 286 | 273 | 7 |         |       |

- Molecule 8 is a protein called Small ribosomal subunit protein eS6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | I     | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1923  | 1200 | 387 | 329 | 7 |         |       |

- Molecule 9 is a protein called Small ribosomal subunit protein eS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | J     | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1530  | 975 | 281 | 273 | 1 |         |       |

- Molecule 10 is a protein called Small ribosomal subunit protein eS8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | K     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1054 | 329 | 291 | 5 |         |       |

- Molecule 11 is a protein called Small ribosomal subunit protein uS4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | L     | 182      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1498  | 952 | 300 | 244 | 2 |         |       |

- Molecule 12 is a protein called Small ribosomal subunit protein eS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | M     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 539 | 148 | 134 | 6 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| M     | -30     | THR      | ALA    | conflict | UNP A0AAG1W9A6 |

- Molecule 13 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | N     | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1296  | 827 | 241 | 221 | 7 |         |       |

- Molecule 14 is a protein called Small ribosomal subunit protein eS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | O     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 958   | 600 | 170 | 179 | 9 |         |       |

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | P     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 16 is a protein called Ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | Q     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1016  | 621 | 199 | 190 | 6 |         |       |

- Molecule 17 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | R     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 704 | 211 | 189 | 7 |         |       |

- Molecule 18 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | S     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 715 | 212 | 193 | 3 |         |       |

- Molecule 19 is a protein called Small ribosomal subunit protein eS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | T     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1019  | 639 | 188 | 187 | 5 |         |       |

- Molecule 20 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | U     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 239 | 199 | 1 |         |       |

- Molecule 21 is a protein called Small ribosomal subunit protein eS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | V     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1113  | 701 | 213 | 196 | 3 |         |       |

- Molecule 22 is a protein called Small ribosomal subunit protein uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | W     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 822   | 514 | 156 | 148 | 4 |         |       |

- Molecule 23 is a protein called Small ribosomal subunit protein eS21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | X     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 619   | 378 | 117 | 119 | 5 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| X     | 3       | SER      | ASN    | conflict | UNP G1TM82 |
| X     | 4       | ASN      | ASP    | conflict | UNP G1TM82 |
| X     | 33      | PRO      | GLN    | conflict | UNP G1TM82 |
| X     | 50      | SER      | PHE    | conflict | UNP G1TM82 |
| X     | 76      | HIS      | ASP    | conflict | UNP G1TM82 |

- Molecule 24 is a protein called Small ribosomal subunit protein uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | Y     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 25 is a protein called Small ribosomal subunit protein uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Z     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1106  | 698 | 220 | 184 | 4 |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | a     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 645 | 198 | 174 | 5 |         |       |

- Molecule 27 is a protein called Small ribosomal subunit protein eS26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | b     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 789   | 491 | 162 | 130 | 6 |         |       |

- Molecule 28 is a protein called Small ribosomal subunit protein eS27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | c     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 659   | 413 | 122 | 116 | 8 |         |       |

- Molecule 29 is a protein called Small ribosomal subunit protein eS28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 29  | d     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 507   | 308 | 102 | 95 | 2 |         |       |

- Molecule 30 is a protein called Small ribosomal subunit protein uS14.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30  | e     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 445   | 278 | 90 | 72 | 5 |         |       |

- Molecule 31 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 31  | f     | 71       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 581   | 367 | 109 | 98 | 7 |         |       |

- Molecule 32 is a protein called Small ribosomal subunit protein RACK1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 32  | g     | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 33 is a protein called Small ribosomal subunit protein eS25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | h     | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 598   | 382 | 111 | 104 | 1 |         |       |

- Molecule 34 is a protein called Small ribosomal subunit protein eS30.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 34  | i     | 59       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 473   | 293 | 104 | 75 | 1 |         |       |

- Molecule 35 is a protein called Small ribosomal subunit protein eS32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | l     | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 240   | 145 | 64 | 28 | 3 |         |       |

- Molecule 36 is a RNA chain called Initiator tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 36  | y     | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1604  | 717 | 298 | 515 | 74 |         |       |

- Molecule 37 is a RNA chain called EMCV IRES.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 37  | z     | 93       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1981  | 885 | 361 | 642 | 93 |         |       |

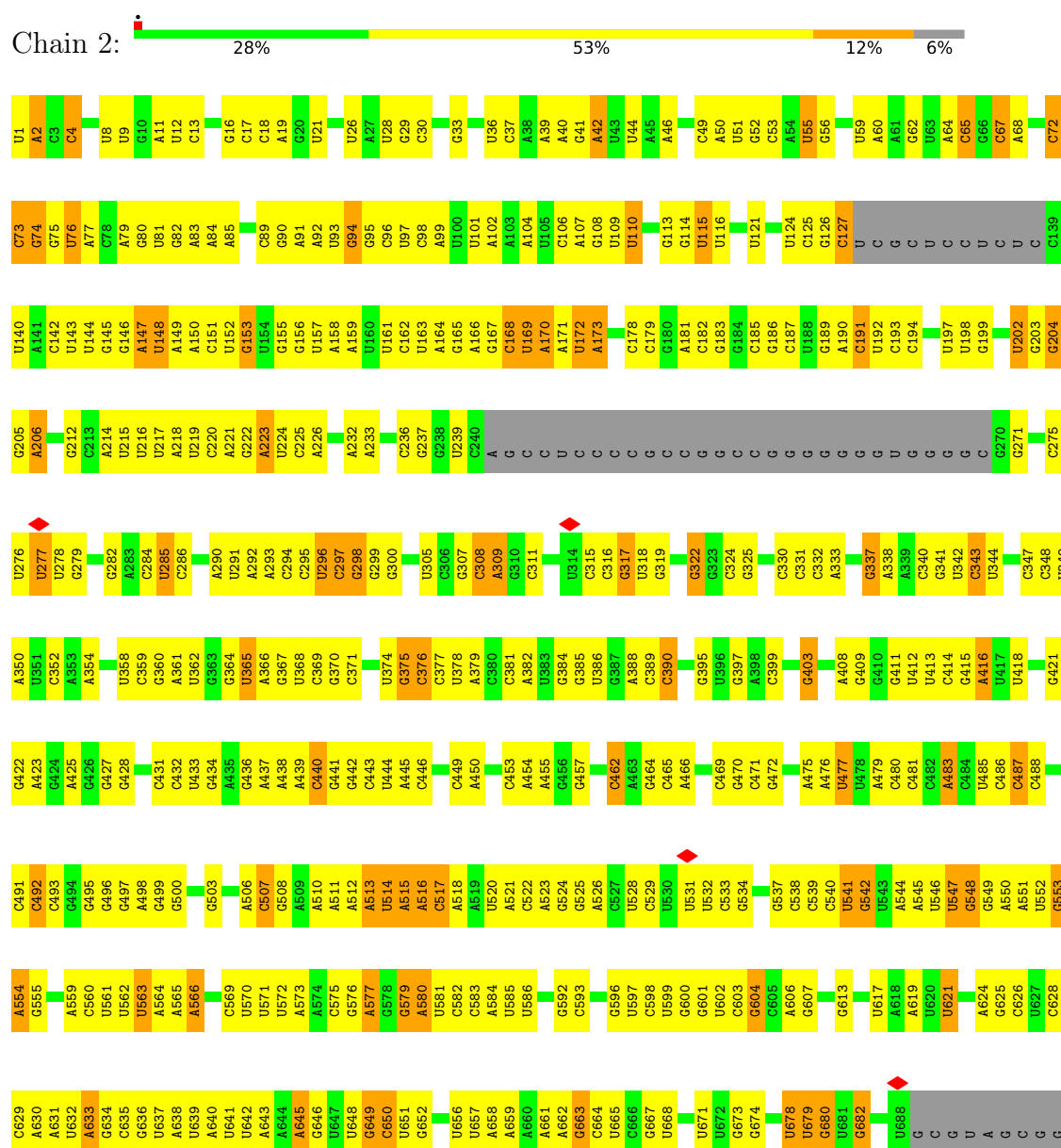
There are 8 discrepancies between the modelled and reference sequences:

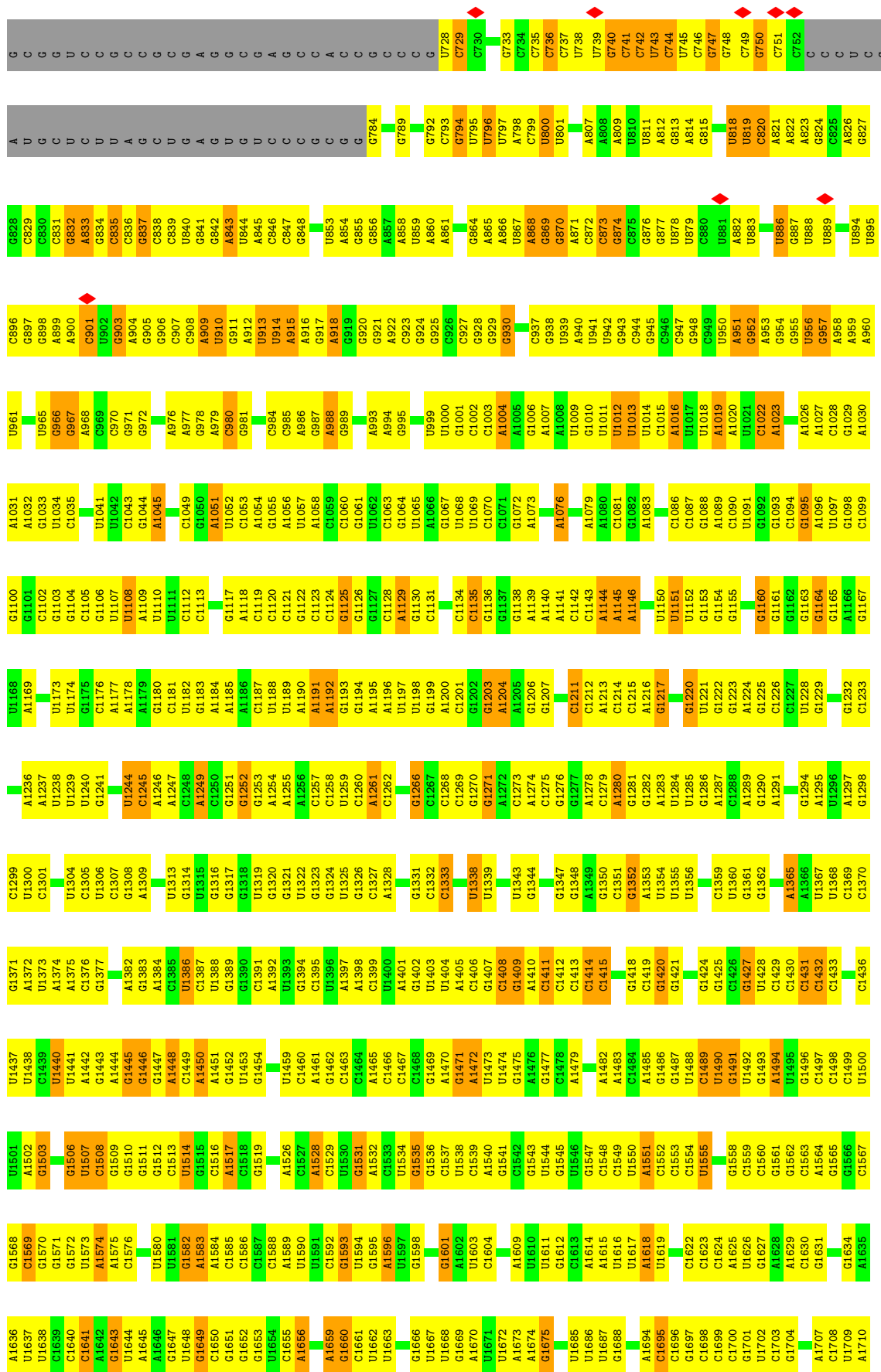
| Chain | Residue | Modelled | Actual | Comment        | Reference    |
|-------|---------|----------|--------|----------------|--------------|
| z     | 831     | A        | -      | expression tag | GB 485965777 |
| z     | 832     | A        | -      | expression tag | GB 485965777 |
| z     | 833     | U        | -      | expression tag | GB 485965777 |
| z     | 834     | A        | -      | expression tag | GB 485965777 |
| z     | 835     | U        | -      | expression tag | GB 485965777 |
| z     | 836     | G        | -      | expression tag | GB 485965777 |
| z     | 837     | G        | -      | expression tag | GB 485965777 |
| z     | 838     | C        | -      | expression tag | GB 485965777 |

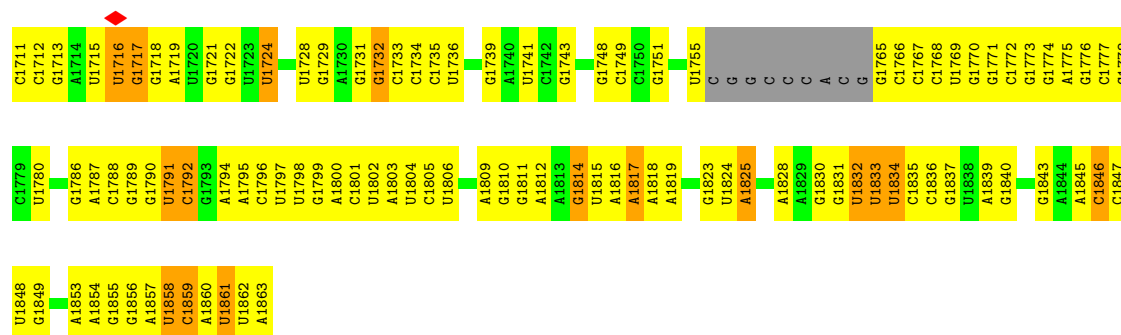
### 3 Residue-property plots

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.

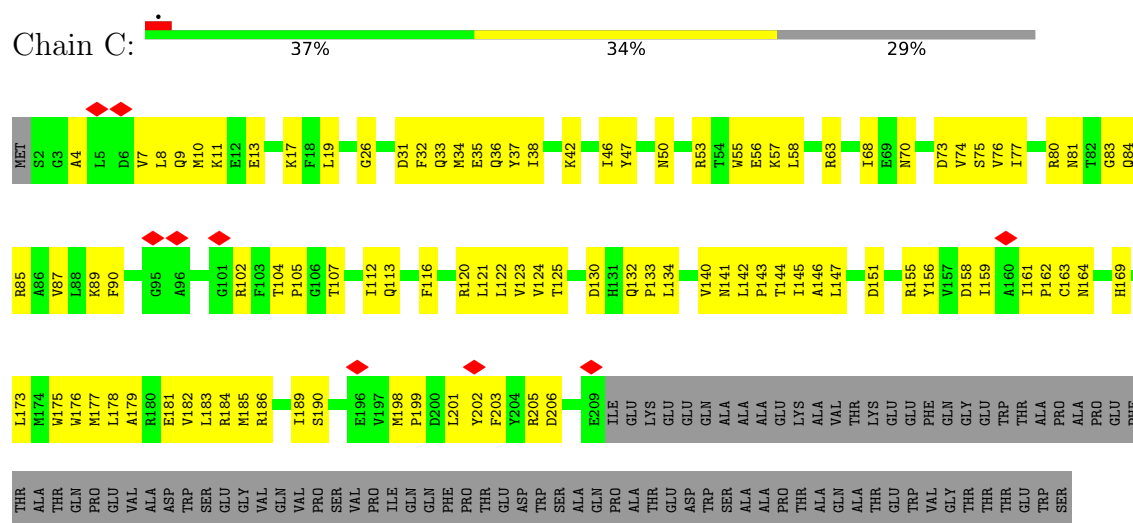
#### • Molecule 1: 18S ribosomal RNA



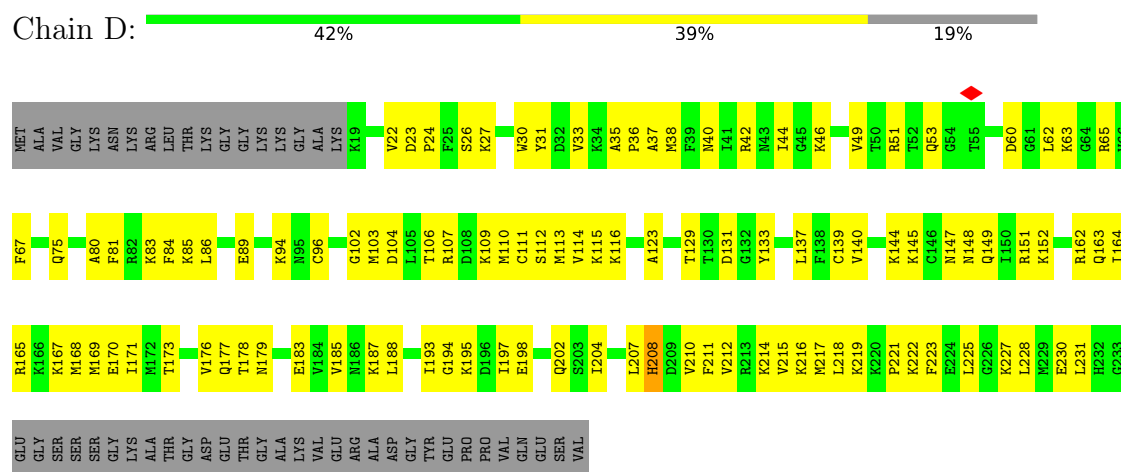




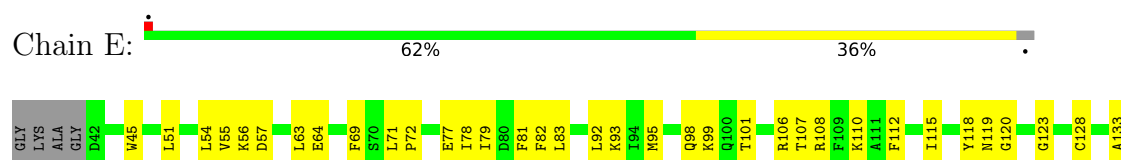
• Molecule 2: Small ribosomal subunit protein uS2

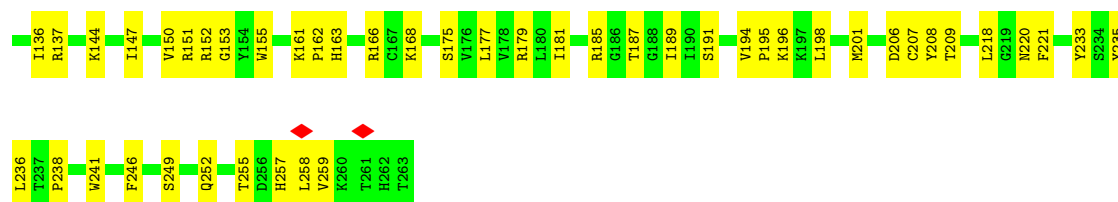


• Molecule 3: Small ribosomal subunit protein eS1

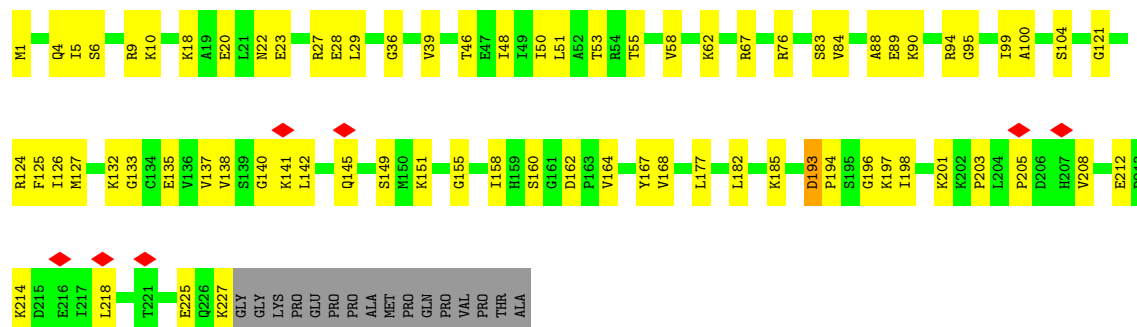


• Molecule 4: Small ribosomal subunit protein uS5





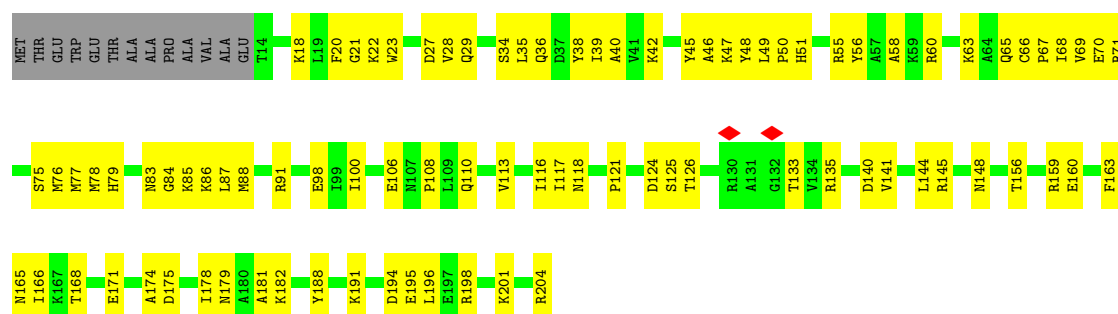
• Molecule 5: Small ribosomal subunit protein uS3



• Molecule 6: Small ribosomal subunit protein eS4

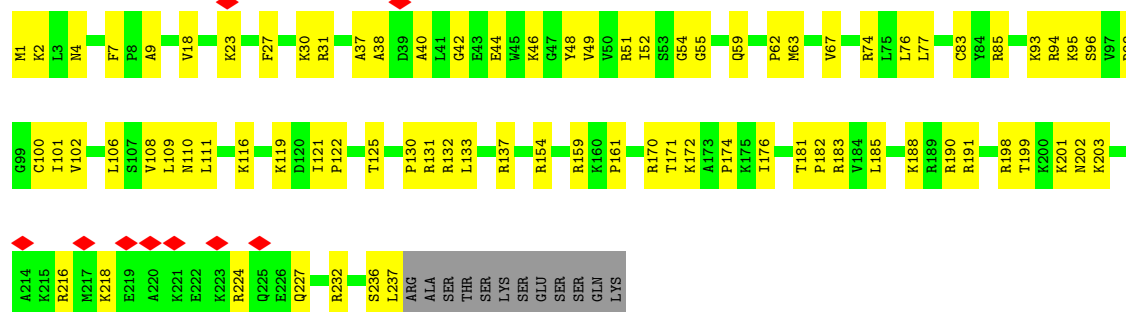


• Molecule 7: Small ribosomal subunit protein uS7



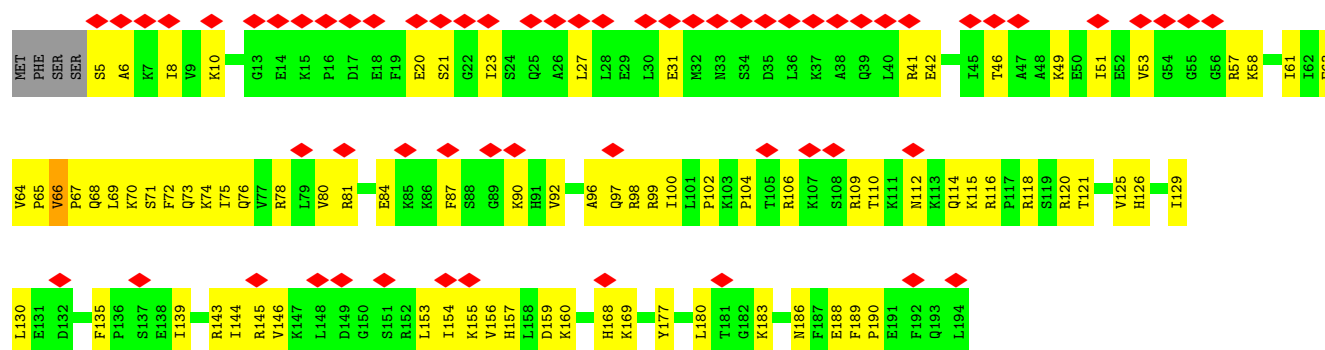
• Molecule 8: Small ribosomal subunit protein eS6

Chain I: 



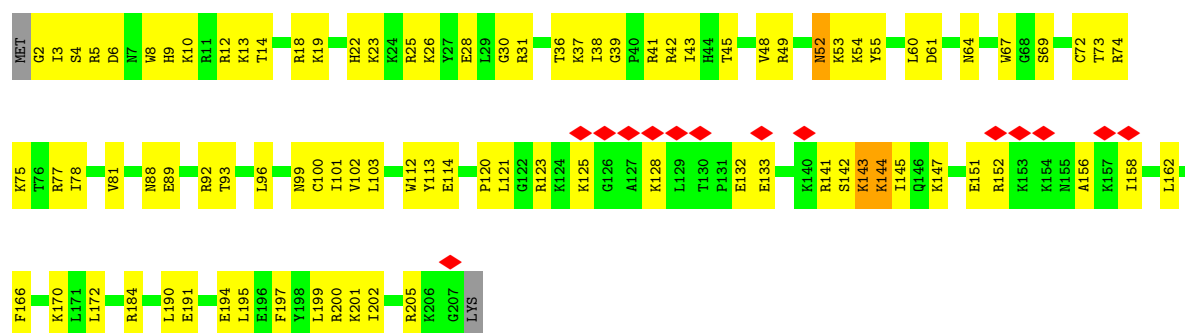
• Molecule 9: Small ribosomal subunit protein eS7

Chain J: 



• Molecule 10: Small ribosomal subunit protein eS8

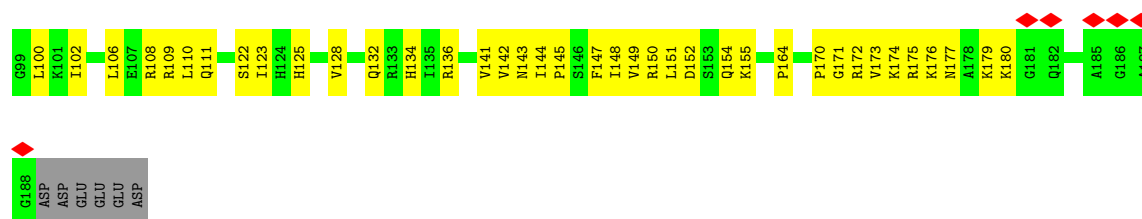
Chain K: 



• Molecule 11: Small ribosomal subunit protein uS4

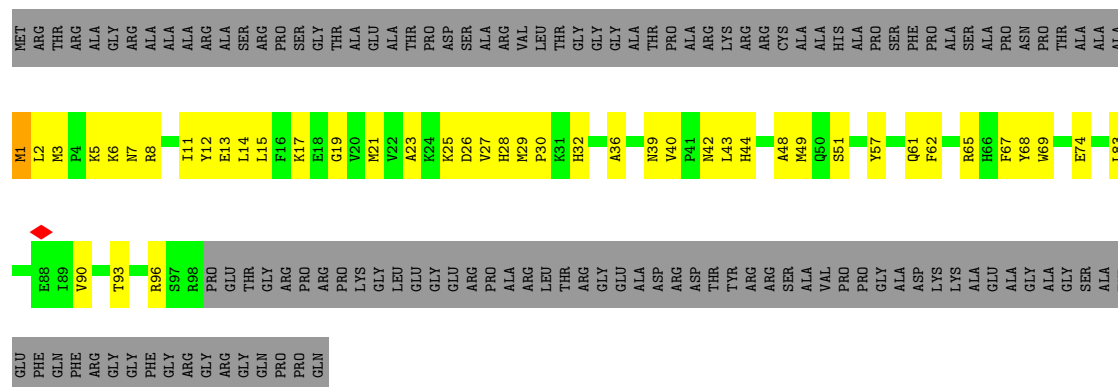
Chain L: 





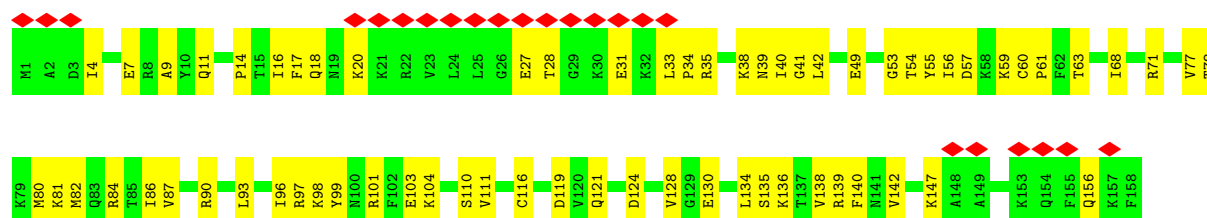
• Molecule 12: Small ribosomal subunit protein eS10

Chain M: 24% 19% 56%



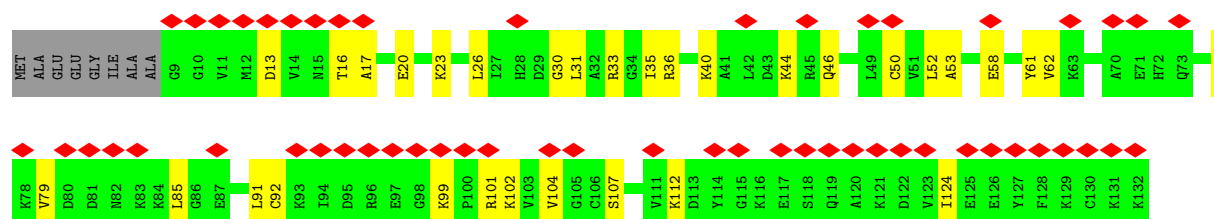
• Molecule 13: Small ribosomal subunit protein uS17

Chain N: 15% 58% 42%



• Molecule 14: Small ribosomal subunit protein eS12

Chain O: 41% 70% 24% 6%



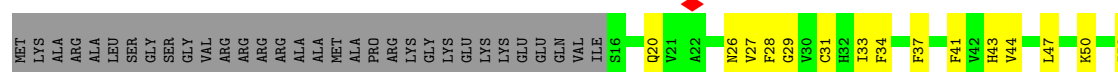
• Molecule 15: Small ribosomal subunit protein uS15

Chain P: 58% 41%





• Molecule 16: Ribosomal protein S14



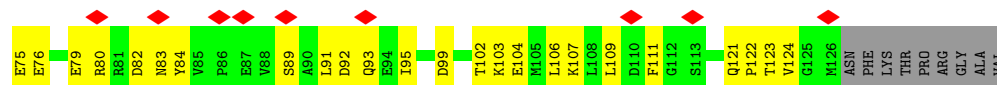
• Molecule 17: Small ribosomal subunit protein uS19



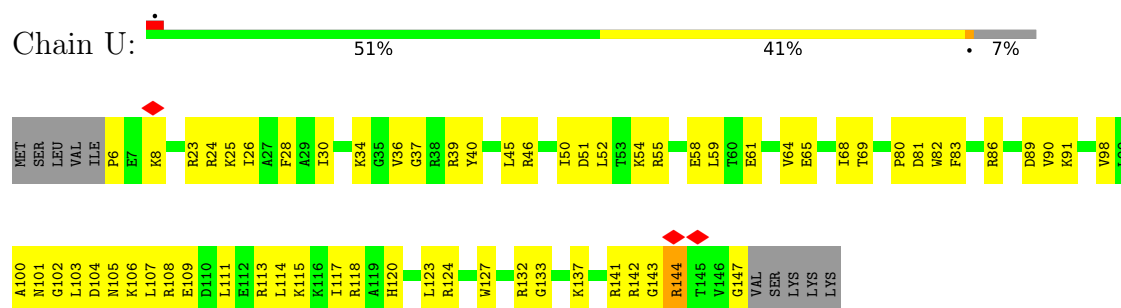
• Molecule 18: Small ribosomal subunit protein uS9



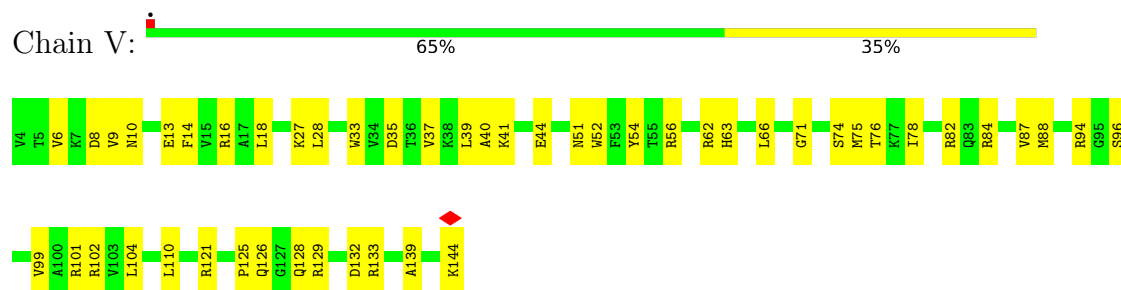
• Molecule 19: Small ribosomal subunit protein eS17



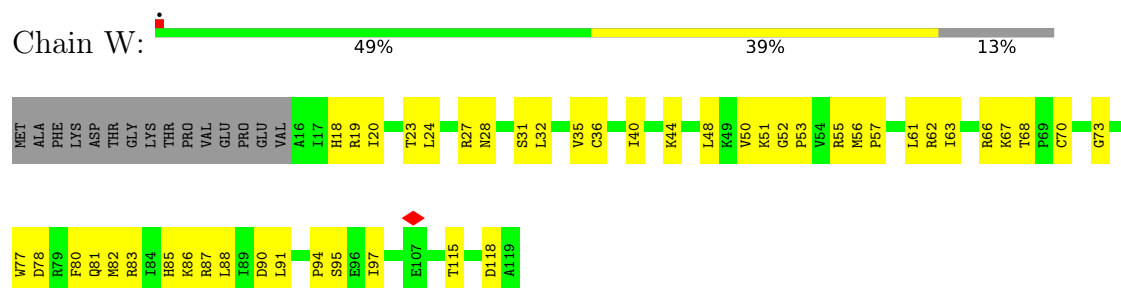
- Molecule 20: Small ribosomal subunit protein uS13



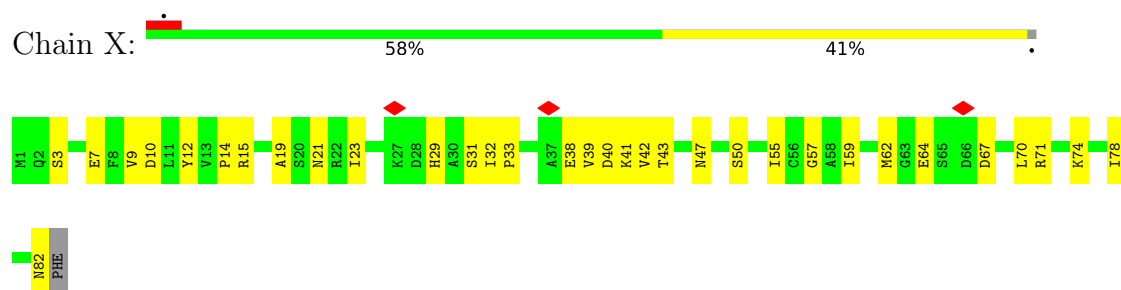
- Molecule 21: Small ribosomal subunit protein eS19



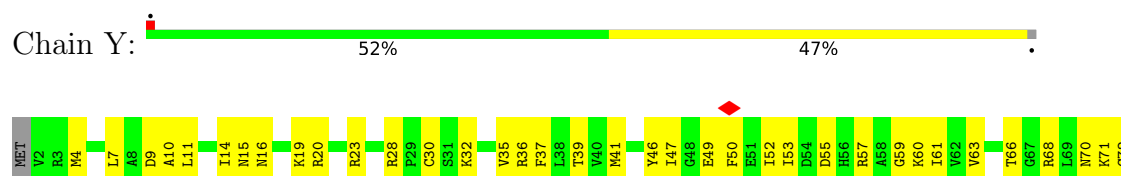
- Molecule 22: Small ribosomal subunit protein uS10

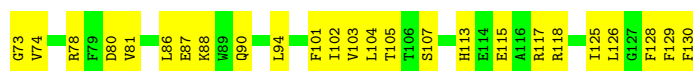


- Molecule 23: Small ribosomal subunit protein eS21



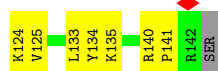
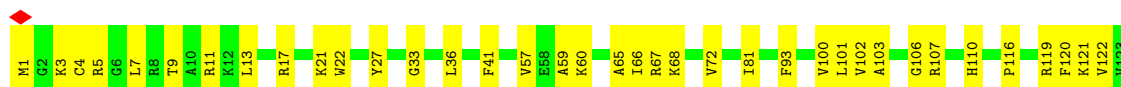
- Molecule 24: Small ribosomal subunit protein uS8





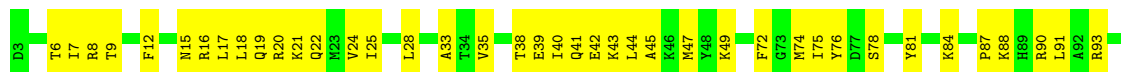
- Molecule 25: Small ribosomal subunit protein uS12

Chain Z: 69% 31%



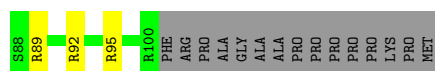
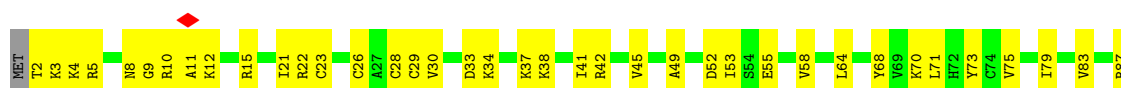
- Molecule 26: 40S ribosomal protein S24

Chain a: 56% 42%



- Molecule 27: Small ribosomal subunit protein eS26

Chain b: 50% 36% 14%



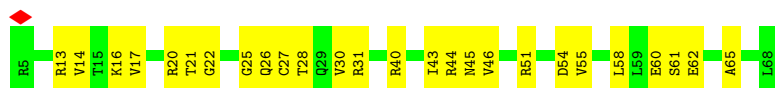
- Molecule 28: Small ribosomal subunit protein eS27

Chain c: 55% 45%



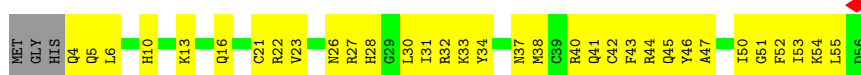
- Molecule 29: Small ribosomal subunit protein eS28

Chain d: 59% 41%



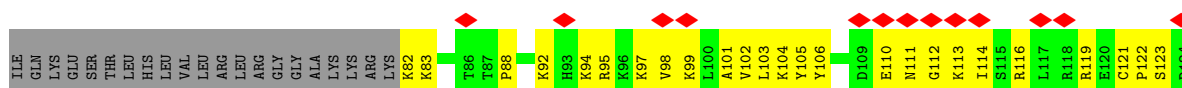
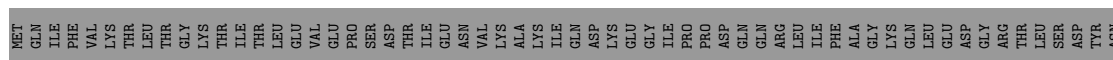
- Molecule 30: Small ribosomal subunit protein uS14

Chain e: 



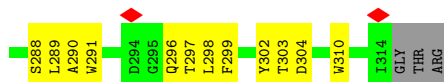
- Molecule 31: Ubiquitin-ribosomal protein eS31 fusion protein

Chain f: 

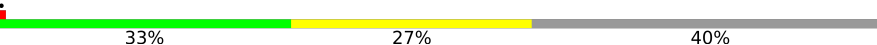


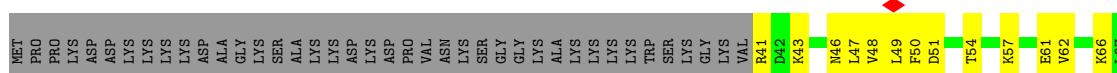
- Molecule 32: Small ribosomal subunit protein RACK1

Chain g: 

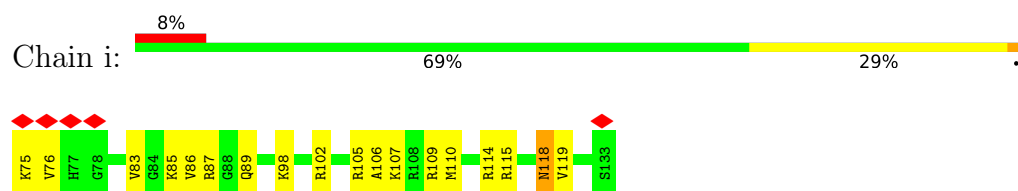


- Molecule 33: Small ribosomal subunit protein eS25

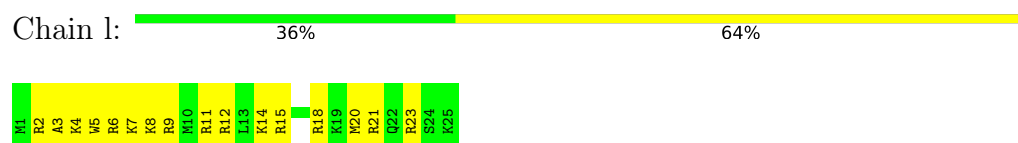
Chain h: 



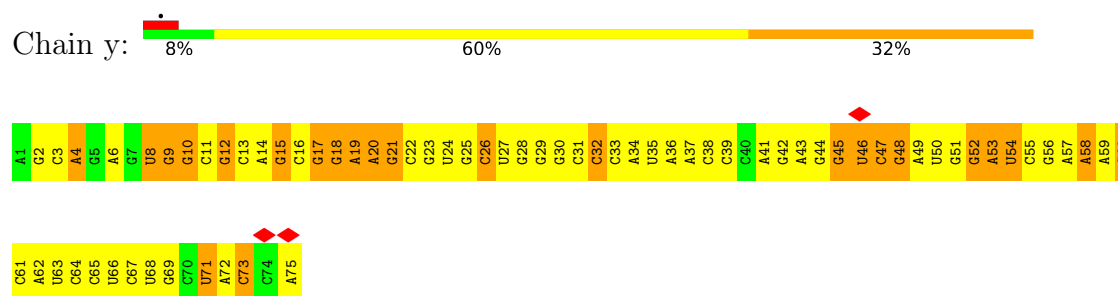
- Molecule 34: Small ribosomal subunit protein eS30



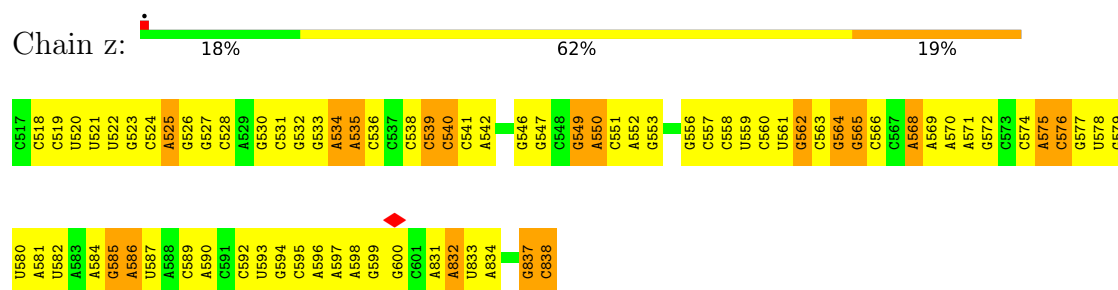
- Molecule 35: Small ribosomal subunit protein eS32



- Molecule 36: Initiator tRNA



- Molecule 37: EMCV IRES



## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, C1                       | Depositor |
| Number of particles used             | 55231                           | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | NONE                            | Depositor |
| Microscope                           | FEI TALOS ARCTICA               | Depositor |
| Voltage (kV)                         | 200                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 55                              | Depositor |
| Minimum defocus (nm)                 | 1250                            | Depositor |
| Maximum defocus (nm)                 | 2750                            | Depositor |
| Magnification                        | 36000                           | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)       | Depositor |
| Maximum map value                    | 0.621                           | Depositor |
| Minimum map value                    | -0.247                          | Depositor |
| Average map value                    | 0.001                           | Depositor |
| Map value standard deviation         | 0.022                           | Depositor |
| Recommended contour level            | 0.0811                          | Depositor |
| Map size ( $\text{\AA}$ )            | 467.99997, 467.99997, 467.99997 | wwPDB     |
| Map dimensions                       | 400, 400, 400                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.17, 1.17, 1.17                | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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   | 2     | 0.12         | 0/41584 | 0.29        | 0/64804       |
| 2   | C     | 0.18         | 0/1679  | 0.47        | 0/2283        |
| 3   | D     | 0.16         | 0/1769  | 0.46        | 0/2367        |
| 4   | E     | 0.19         | 0/1757  | 0.43        | 0/2371        |
| 5   | F     | 0.14         | 0/1792  | 0.44        | 2/2412 (0.1%) |
| 6   | G     | 0.15         | 0/2125  | 0.39        | 0/2856        |
| 7   | H     | 0.16         | 0/1531  | 0.39        | 0/2059        |
| 8   | I     | 0.11         | 0/1945  | 0.35        | 0/2587        |
| 9   | J     | 0.17         | 0/1553  | 0.45        | 0/2079        |
| 10  | K     | 0.14         | 0/1708  | 0.46        | 2/2278 (0.1%) |
| 11  | L     | 0.15         | 0/1522  | 0.41        | 0/2031        |
| 12  | M     | 0.16         | 0/851   | 0.50        | 2/1147 (0.2%) |
| 13  | N     | 0.16         | 0/1319  | 0.41        | 0/1761        |
| 14  | O     | 0.09         | 0/968   | 0.32        | 0/1296        |
| 15  | P     | 0.13         | 0/1232  | 0.39        | 0/1656        |
| 16  | Q     | 0.14         | 0/1029  | 0.42        | 0/1380        |
| 17  | R     | 0.14         | 0/1132  | 0.46        | 0/1510        |
| 18  | S     | 0.13         | 0/1141  | 0.38        | 0/1528        |
| 19  | T     | 0.15         | 0/1031  | 0.46        | 0/1383        |
| 20  | U     | 0.15         | 0/1190  | 0.47        | 0/1592        |
| 21  | V     | 0.13         | 0/1133  | 0.35        | 0/1517        |
| 22  | W     | 0.12         | 0/832   | 0.33        | 0/1117        |
| 23  | X     | 0.13         | 0/626   | 0.42        | 0/839         |
| 24  | Y     | 0.19         | 0/1051  | 0.45        | 0/1406        |
| 25  | Z     | 0.14         | 0/1124  | 0.41        | 0/1500        |
| 26  | a     | 0.20         | 0/1038  | 0.57        | 4/1377 (0.3%) |
| 27  | b     | 0.21         | 0/802   | 0.44        | 0/1076        |
| 28  | c     | 0.22         | 0/673   | 0.50        | 2/902 (0.2%)  |
| 29  | d     | 0.14         | 0/509   | 0.41        | 0/680         |
| 30  | e     | 0.15         | 0/455   | 0.46        | 0/603         |
| 31  | f     | 0.13         | 0/593   | 0.41        | 0/786         |
| 32  | g     | 0.11         | 0/2493  | 0.34        | 0/3394        |
| 33  | h     | 0.15         | 0/604   | 0.34        | 0/810         |
| 34  | i     | 0.12         | 0/478   | 0.57        | 2/628 (0.3%)  |

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 35  | l     | 0.14         | 0/241   | 0.41        | 0/305            |
| 36  | y     | 0.13         | 0/1795  | 0.30        | 0/2798           |
| 37  | z     | 0.11         | 0/2213  | 0.27        | 0/3442           |
| All | All   | 0.13         | 0/85518 | 0.35        | 14/124560 (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 |
|-----|-------|---------------------|---------------------|
| 3   | D     | 0                   | 1                   |
| 9   | J     | 0                   | 1                   |
| 18  | S     | 0                   | 1                   |
| 26  | a     | 0                   | 2                   |
| All | All   | 0                   | 5                   |

There are no bond length outliers.

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 12  | M     | 1   | MET  | CA-C-N   | 8.63  | 137.23      | 121.70   |
| 12  | M     | 1   | MET  | C-N-CA   | 8.63  | 137.23      | 121.70   |
| 5   | F     | 197 | LYS  | CA-C-N   | 7.29  | 134.83      | 121.70   |
| 5   | F     | 197 | LYS  | C-N-CA   | 7.29  | 134.83      | 121.70   |
| 34  | i     | 118 | ASN  | CA-C-N   | 6.48  | 133.36      | 121.70   |
| 34  | i     | 118 | ASN  | C-N-CA   | 6.48  | 133.36      | 121.70   |
| 28  | c     | 81  | ARG  | CA-C-N   | 6.45  | 133.31      | 121.70   |
| 28  | c     | 81  | ARG  | C-N-CA   | 6.45  | 133.31      | 121.70   |
| 26  | a     | 42  | GLU  | CA-CB-CG | 5.86  | 125.81      | 114.10   |
| 10  | K     | 143 | LYS  | CA-C-N   | 5.27  | 131.60      | 121.54   |
| 10  | K     | 143 | LYS  | C-N-CA   | 5.27  | 131.60      | 121.54   |
| 26  | a     | 42  | GLU  | N-CA-CB  | 5.25  | 117.93      | 110.16   |
| 26  | a     | 101 | LYS  | CA-C-N   | -5.03 | 116.45      | 122.44   |
| 26  | a     | 101 | LYS  | C-N-CA   | -5.03 | 116.45      | 122.44   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | D     | 208 | HIS  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 9   | J     | 66  | VAL  | Peptide |
| 18  | S     | 43  | GLU  | Peptide |
| 26  | a     | 102 | THR  | Peptide |
| 26  | a     | 103 | SER  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 2     | 37194 | 0        | 18795    | 1207    | 0            |
| 2   | C     | 1642  | 0        | 1646     | 97      | 0            |
| 3   | D     | 1741  | 0        | 1815     | 82      | 0            |
| 4   | E     | 1721  | 0        | 1812     | 69      | 0            |
| 5   | F     | 1764  | 0        | 1863     | 58      | 0            |
| 6   | G     | 2083  | 0        | 2189     | 98      | 0            |
| 7   | H     | 1509  | 0        | 1563     | 75      | 0            |
| 8   | I     | 1923  | 0        | 2088     | 63      | 0            |
| 9   | J     | 1530  | 0        | 1627     | 83      | 0            |
| 10  | K     | 1679  | 0        | 1760     | 77      | 0            |
| 11  | L     | 1498  | 0        | 1608     | 72      | 0            |
| 12  | M     | 827   | 0        | 854      | 35      | 0            |
| 13  | N     | 1296  | 0        | 1374     | 59      | 0            |
| 14  | O     | 958   | 0        | 993      | 26      | 0            |
| 15  | P     | 1208  | 0        | 1294     | 58      | 0            |
| 16  | Q     | 1016  | 0        | 1039     | 47      | 0            |
| 17  | R     | 1111  | 0        | 1168     | 67      | 0            |
| 18  | S     | 1123  | 0        | 1193     | 60      | 0            |
| 19  | T     | 1019  | 0        | 1075     | 56      | 0            |
| 20  | U     | 1172  | 0        | 1226     | 67      | 0            |
| 21  | V     | 1113  | 0        | 1149     | 37      | 0            |
| 22  | W     | 822   | 0        | 887      | 43      | 0            |
| 23  | X     | 619   | 0        | 622      | 35      | 0            |
| 24  | Y     | 1034  | 0        | 1080     | 70      | 0            |
| 25  | Z     | 1106  | 0        | 1179     | 41      | 0            |
| 26  | a     | 1022  | 0        | 1084     | 54      | 0            |
| 27  | b     | 789   | 0        | 839      | 45      | 0            |
| 28  | c     | 659   | 0        | 683      | 32      | 0            |
| 29  | d     | 507   | 0        | 536      | 21      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 30  | e     | 445   | 0        | 442      | 36      | 0            |
| 31  | f     | 581   | 0        | 599      | 39      | 0            |
| 32  | g     | 2436  | 0        | 2393     | 95      | 0            |
| 33  | h     | 598   | 0        | 656      | 30      | 0            |
| 34  | i     | 473   | 0        | 524      | 17      | 0            |
| 35  | l     | 240   | 0        | 289      | 17      | 0            |
| 36  | y     | 1604  | 0        | 816      | 61      | 0            |
| 37  | z     | 1981  | 0        | 1011     | 74      | 0            |
| All | All   | 80043 | 0        | 61771    | 2688    | 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 19.

All (2688) 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) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:2:124:U:H3    | 1:2:330:C:N4      | 1.55                     | 1.02              |
| 1:2:1704:G:H1   | 1:2:1818:A:H61    | 1.00                     | 1.00              |
| 1:2:1751:G:H1   | 1:2:1769:U:H3     | 1.07                     | 0.97              |
| 1:2:432:C:N4    | 1:2:439:A:H62     | 1.62                     | 0.96              |
| 1:2:432:C:H42   | 1:2:439:A:N6      | 1.64                     | 0.94              |
| 1:2:1743:G:H1   | 1:2:1780:U:H3     | 1.15                     | 0.92              |
| 1:2:1836:C:OP2  | 35:l:4:LYS:NZ     | 2.03                     | 0.91              |
| 1:2:874:G:H1    | 1:2:904:A:H2      | 1.04                     | 0.91              |
| 1:2:1647:G:H1   | 1:2:1667:U:H3     | 0.98                     | 0.91              |
| 1:2:116:U:H3    | 1:2:337:G:H1      | 0.99                     | 0.90              |
| 10:K:142:SER:HA | 10:K:145:ILE:HG13 | 1.54                     | 0.89              |
| 9:J:63:PHE:HB3  | 9:J:97:GLN:HB2    | 1.55                     | 0.88              |
| 6:G:182:MET:HE1 | 6:G:192:ILE:HG12  | 1.55                     | 0.87              |
| 1:2:1704:G:H1   | 1:2:1818:A:N6     | 1.71                     | 0.87              |
| 1:2:149:A:N6    | 1:2:169:U:C2      | 2.43                     | 0.86              |
| 1:2:1394:G:H1   | 1:2:1444:A:H61    | 1.19                     | 0.86              |
| 10:K:144:LYS:H  | 10:K:147:LYS:HE2  | 1.40                     | 0.85              |
| 2:C:130:ASP:HB3 | 2:C:133:PRO:HG2   | 1.60                     | 0.84              |
| 12:M:29:MET:HE2 | 12:M:32:HIS:HA    | 1.57                     | 0.84              |
| 1:2:847:C:H5''  | 1:2:848:G:H5'     | 1.60                     | 0.84              |
| 1:2:1472:A:N7   | 19:T:3:ARG:NH2    | 2.26                     | 0.83              |
| 2:C:38:ILE:HD11 | 2:C:47:TYR:HB3    | 1.60                     | 0.83              |
| 1:2:874:G:N1    | 1:2:904:A:C2      | 2.45                     | 0.83              |
| 1:2:146:G:H1    | 1:2:173:A:H61     | 1.23                     | 0.83              |
| 1:2:1095:G:H1   | 1:2:1129:A:H61    | 1.24                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:483:A:H61     | 1:2:500:G:H1'     | 1.43                     | 0.82              |
| 2:C:203:PHE:O     | 2:C:205:ARG:NH2   | 2.13                     | 0.82              |
| 1:2:189:G:H3'     | 10:K:141:ARG:HH12 | 1.44                     | 0.81              |
| 1:2:826:A:OP2     | 1:2:842:G:N2      | 2.13                     | 0.81              |
| 17:R:13:ARG:HD2   | 17:R:14:LYS:HB2   | 1.62                     | 0.81              |
| 20:U:46:ARG:HD2   | 21:V:35:ASP:HB3   | 1.59                     | 0.81              |
| 1:2:940:A:H61     | 1:2:978:G:H1      | 1.27                     | 0.81              |
| 17:R:17:TYR:HA    | 20:U:91:LYS:HA    | 1.61                     | 0.81              |
| 1:2:1226:C:HO2'   | 1:2:1660:G:H1     | 1.28                     | 0.81              |
| 1:2:124:U:H3      | 1:2:330:C:H42     | 0.85                     | 0.81              |
| 1:2:1012:U:OP1    | 28:c:20:LYS:NZ    | 2.15                     | 0.80              |
| 1:2:1188:U:OP2    | 25:Z:119:ARG:NH2  | 2.13                     | 0.80              |
| 1:2:953:A:H3'     | 1:2:954:G:H21     | 1.45                     | 0.80              |
| 1:2:958:A:H5''    | 16:Q:66:ARG:HD2   | 1.63                     | 0.80              |
| 1:2:1644:U:H3     | 1:2:1670:A:H2     | 1.27                     | 0.80              |
| 28:c:42:LYS:HZ3   | 28:c:57:VAL:H     | 1.30                     | 0.80              |
| 11:L:78:LEU:HD13  | 11:L:92:MET:HE1   | 1.62                     | 0.80              |
| 1:2:1652:G:H1     | 1:2:1662:U:H3     | 1.30                     | 0.79              |
| 1:2:1139:A:O3'    | 1:2:1351:C:N4     | 2.16                     | 0.79              |
| 1:2:668:U:H3      | 1:2:1023:A:H62    | 1.27                     | 0.78              |
| 9:J:78:ARG:HH12   | 9:J:81:ARG:HH11   | 1.29                     | 0.78              |
| 9:J:84:GLU:HG3    | 9:J:92:VAL:HG12   | 1.66                     | 0.78              |
| 25:Z:101:LEU:HD12 | 25:Z:124:LYS:HD2  | 1.66                     | 0.78              |
| 1:2:432:C:H42     | 1:2:439:A:H62     | 0.83                     | 0.77              |
| 2:C:122:LEU:HD21  | 2:C:144:THR:HG22  | 1.67                     | 0.77              |
| 1:2:1450:A:H5''   | 19:T:3:ARG:HH12   | 1.50                     | 0.77              |
| 1:2:1672:U:OP1    | 7:H:71:ARG:NH2    | 2.17                     | 0.77              |
| 27:b:89:ARG:HA    | 27:b:92:ARG:HE    | 1.49                     | 0.77              |
| 1:2:59:U:H5'      | 1:2:493:C:H41     | 1.50                     | 0.76              |
| 1:2:1408:C:H2'    | 1:2:1409:G:C8     | 2.21                     | 0.76              |
| 1:2:650:C:H5'     | 25:Z:13:LEU:HD11  | 1.66                     | 0.76              |
| 1:2:1281:G:H22    | 31:f:104:LYS:HG2  | 1.51                     | 0.75              |
| 3:D:139:CYS:HA    | 3:D:212:VAL:HA    | 1.65                     | 0.75              |
| 6:G:10:LYS:HE3    | 6:G:13:ALA:HB2    | 1.67                     | 0.75              |
| 1:2:1414:C:N4     | 1:2:1421:G:OP2    | 2.19                     | 0.75              |
| 37:z:589:C:H2'    | 37:z:590:A:H8     | 1.52                     | 0.75              |
| 14:O:36:ARG:NH2   | 31:f:129:GLY:O    | 2.20                     | 0.75              |
| 1:2:1320:G:N2     | 1:2:1500:U:O2     | 2.20                     | 0.75              |
| 1:2:1519:G:OP2    | 20:U:141:ARG:NH1  | 2.20                     | 0.75              |
| 10:K:113:TYR:HB3  | 10:K:121:LEU:HD21 | 1.69                     | 0.75              |
| 19:T:79:GLU:HA    | 19:T:82:ASP:HB3   | 1.67                     | 0.75              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 19:T:41:ILE:HG12 | 19:T:47:ARG:HB2   | 1.68                     | 0.75              |
| 1:2:826:A:N6     | 1:2:840:U:O2      | 2.19                     | 0.74              |
| 17:R:94:VAL:HG12 | 17:R:107:ILE:HD11 | 1.67                     | 0.74              |
| 1:2:146:G:H1     | 1:2:173:A:N6      | 1.85                     | 0.74              |
| 1:2:1320:G:H1    | 1:2:1500:U:H3     | 1.32                     | 0.74              |
| 1:2:1418:G:H2'   | 1:2:1419:C:H2'    | 1.70                     | 0.74              |
| 32:g:256:ILE:HB  | 32:g:270:LEU:HB2  | 1.70                     | 0.74              |
| 32:g:5:MET:HE3   | 32:g:6:THR:H      | 1.52                     | 0.74              |
| 1:2:94:G:OP1     | 6:G:8:HIS:ND1     | 2.20                     | 0.73              |
| 1:2:309:A:H2     | 1:2:322:G:H22     | 1.34                     | 0.73              |
| 1:2:1083:A:OP1   | 27:b:3:LYS:NZ     | 2.15                     | 0.73              |
| 24:Y:11:LEU:HD21 | 24:Y:74:VAL:HB    | 1.70                     | 0.73              |
| 25:Z:17:ARG:O    | 25:Z:21:LYS:HB2   | 1.88                     | 0.73              |
| 1:2:1490:U:H4'   | 1:2:1491:G:H5''   | 1.69                     | 0.73              |
| 10:K:194:GLU:OE1 | 13:N:18:GLN:NE2   | 2.21                     | 0.73              |
| 13:N:16:ILE:HD11 | 13:N:34:PRO:HG2   | 1.70                     | 0.73              |
| 21:V:10:ASN:H    | 21:V:144:LYS:HE2  | 1.52                     | 0.73              |
| 1:2:551:A:O2'    | 11:L:132:GLN:NE2  | 2.21                     | 0.73              |
| 1:2:800:U:H3     | 1:2:855:G:H1      | 1.36                     | 0.73              |
| 1:2:1054:A:OP1   | 36:y:37:A:O2'     | 2.07                     | 0.73              |
| 3:D:65:ARG:HG2   | 16:Q:50:LYS:HD3   | 1.69                     | 0.73              |
| 26:a:39:GLU:OE1  | 26:a:43:LYS:NZ    | 2.21                     | 0.73              |
| 6:G:197:ASN:HD22 | 6:G:209:HIS:HB2   | 1.52                     | 0.72              |
| 1:2:77:A:H4'     | 8:I:176:ILE:HD12  | 1.71                     | 0.72              |
| 21:V:62:ARG:HH12 | 21:V:66:LEU:HD11  | 1.54                     | 0.72              |
| 20:U:23:ARG:NH2  | 33:h:46:ASN:O     | 2.22                     | 0.72              |
| 1:2:1223:G:H1    | 1:2:1526:A:H61    | 1.38                     | 0.72              |
| 2:C:37:TYR:OH    | 2:C:57:LYS:NZ     | 2.17                     | 0.72              |
| 6:G:45:ILE:HG22  | 6:G:61:VAL:HG11   | 1.72                     | 0.72              |
| 1:2:814:A:OP1    | 11:L:80:ARG:NH2   | 2.21                     | 0.72              |
| 1:2:1284:U:H3    | 1:2:1307:C:H42    | 1.35                     | 0.72              |
| 2:C:122:LEU:HD13 | 2:C:124:VAL:HG23  | 1.71                     | 0.72              |
| 10:K:36:THR:HG23 | 10:K:96:LEU:HB2   | 1.71                     | 0.71              |
| 22:W:81:GLN:HB2  | 30:e:55:LEU:HD21  | 1.71                     | 0.71              |
| 1:2:645:A:H4'    | 1:2:646:G:H3'     | 1.71                     | 0.71              |
| 20:U:26:ILE:HG12 | 20:U:59:LEU:HD11  | 1.72                     | 0.71              |
| 1:2:874:G:N1     | 1:2:904:A:H2      | 1.81                     | 0.71              |
| 1:2:1651:G:H1    | 1:2:1663:U:H3     | 1.36                     | 0.71              |
| 25:Z:101:LEU:HB2 | 25:Z:124:LYS:HB2  | 1.72                     | 0.71              |
| 18:S:85:ARG:HH12 | 18:S:117:ARG:HD3  | 1.55                     | 0.71              |
| 1:2:1519:G:O2'   | 36:y:29:G:OP1     | 2.07                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:842:G:H2'    | 6:G:19:MET:HE1    | 1.72                     | 0.71              |
| 1:2:1645:A:H5''  | 18:S:139:ALA:HB2  | 1.72                     | 0.71              |
| 3:D:83:LYS:HD3   | 3:D:106:THR:HG23  | 1.73                     | 0.71              |
| 7:H:201:LYS:HA   | 7:H:204:ARG:HG2   | 1.73                     | 0.71              |
| 1:2:275:C:N3     | 1:2:887:G:O2'     | 2.24                     | 0.70              |
| 9:J:143:ARG:HB2  | 9:J:155:LYS:HB2   | 1.71                     | 0.70              |
| 31:f:121:CYS:HB3 | 31:f:132:MET:HB2  | 1.73                     | 0.70              |
| 1:2:795:U:OP2    | 9:J:112:ASN:ND2   | 2.24                     | 0.70              |
| 11:L:50:LEU:HD13 | 11:L:102:ILE:HD13 | 1.72                     | 0.70              |
| 7:H:49:LEU:HD23  | 18:S:49:TYR:HB3   | 1.72                     | 0.70              |
| 26:a:87:PRO:HD2  | 26:a:90:ARG:HD2   | 1.73                     | 0.70              |
| 33:h:62:VAL:HG11 | 33:h:96:LEU:HB3   | 1.72                     | 0.70              |
| 33:h:80:ARG:HB3  | 33:h:83:LEU:HB2   | 1.73                     | 0.70              |
| 8:I:121:ILE:HD12 | 8:I:122:PRO:HD2   | 1.73                     | 0.70              |
| 16:Q:34:PHE:HB3  | 16:Q:41:PHE:HB2   | 1.73                     | 0.70              |
| 1:2:4:C:H1'      | 11:L:18:ARG:HH22  | 1.56                     | 0.70              |
| 1:2:1060:C:OP1   | 16:Q:149:ARG:NH2  | 2.24                     | 0.70              |
| 11:L:81:LEU:HB3  | 11:L:87:LEU:HD13  | 1.73                     | 0.70              |
| 1:2:1072:G:O6    | 1:2:1073:A:N6     | 2.24                     | 0.70              |
| 1:2:865:A:C6     | 9:J:114:GLN:HB3   | 2.27                     | 0.70              |
| 1:2:1347:G:H2'   | 1:2:1348:G:H8     | 1.56                     | 0.70              |
| 22:W:51:LYS:HD2  | 22:W:90:ASP:HB3   | 1.74                     | 0.70              |
| 1:2:914:U:O2'    | 24:Y:57:ARG:NH1   | 2.25                     | 0.69              |
| 1:2:924:G:H1     | 1:2:1009:U:H3     | 1.38                     | 0.69              |
| 1:2:53:C:OP1     | 26:a:112:ASN:ND2  | 2.25                     | 0.69              |
| 1:2:869:G:HO2'   | 1:2:870:G:H8      | 1.41                     | 0.69              |
| 17:R:15:PHE:HB3  | 20:U:91:LYS:HB3   | 1.75                     | 0.69              |
| 1:2:1832:U:H1'   | 16:Q:150:ARG:HE   | 1.57                     | 0.69              |
| 4:E:79:ILE:O     | 4:E:83:LEU:HB2    | 1.92                     | 0.69              |
| 5:F:193:ASP:HB3  | 5:F:194:PRO:HD3   | 1.74                     | 0.69              |
| 1:2:365:U:H2'    | 1:2:366:A:C8      | 2.28                     | 0.69              |
| 1:2:514:U:O2'    | 1:2:515:A:OP2     | 2.10                     | 0.69              |
| 1:2:1259:U:H1'   | 30:e:16:GLN:HE21  | 1.58                     | 0.69              |
| 1:2:1537:C:OP1   | 21:V:62:ARG:NH2   | 2.23                     | 0.69              |
| 1:2:1709:U:H2'   | 1:2:1710:A:C8     | 2.27                     | 0.69              |
| 1:2:76:U:H4'     | 8:I:154:ARG:HA    | 1.74                     | 0.69              |
| 1:2:1266:G:H1    | 1:2:1507:U:H3     | 1.41                     | 0.69              |
| 1:2:1474:U:H2'   | 1:2:1475:G:C8     | 2.28                     | 0.69              |
| 6:G:11:ARG:HG3   | 6:G:20:LEU:HD23   | 1.74                     | 0.69              |
| 2:C:31:ASP:HB3   | 2:C:34:MET:HB2    | 1.75                     | 0.69              |
| 36:y:48:G:N2     | 37:z:550:A:O2'    | 2.26                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 32:g:207:CYS:HB2 | 32:g:219:TRP:HB2  | 1.74                     | 0.68              |
| 37:z:518:C:H2'   | 37:z:519:C:C6     | 2.28                     | 0.68              |
| 3:D:40:ASN:OD1   | 3:D:75:GLN:NE2    | 2.26                     | 0.68              |
| 10:K:12:ARG:HG2  | 10:K:13:LYS:H     | 1.58                     | 0.68              |
| 28:c:33:MET:HE1  | 28:c:48:SER:HA    | 1.76                     | 0.68              |
| 1:2:1013:U:OP2   | 15:P:55:ARG:NH1   | 2.26                     | 0.68              |
| 1:2:1095:G:H1    | 1:2:1129:A:N6     | 1.92                     | 0.68              |
| 18:S:146:ARG:NH1 | 36:y:34:A:OP2     | 2.25                     | 0.68              |
| 25:Z:140:ARG:NH1 | 25:Z:141:PRO:O    | 2.25                     | 0.68              |
| 1:2:294:C:O2     | 10:K:184:ARG:NH1  | 2.25                     | 0.68              |
| 1:2:1732:G:O6    | 1:2:1791:U:O2     | 2.10                     | 0.68              |
| 9:J:75:ILE:HG23  | 9:J:76:GLN:H      | 1.59                     | 0.68              |
| 12:M:3:MET:HE2   | 12:M:8:ARG:HG3    | 1.76                     | 0.68              |
| 36:y:29:G:H2'    | 36:y:30:G:C8      | 2.27                     | 0.68              |
| 1:2:1094:C:H2'   | 1:2:1095:G:C8     | 2.27                     | 0.68              |
| 24:Y:53:ILE:HB   | 24:Y:60:LYS:HB2   | 1.74                     | 0.68              |
| 1:2:833:A:H5''   | 26:a:47:MET:HE1   | 1.75                     | 0.68              |
| 36:y:3:C:H2'     | 36:y:4:A:C8       | 2.29                     | 0.68              |
| 1:2:668:U:OP2    | 1:2:1022:C:N4     | 2.26                     | 0.68              |
| 6:G:192:ILE:HG13 | 6:G:243:GLY:HA3   | 1.76                     | 0.68              |
| 11:L:50:LEU:HD21 | 11:L:54:ARG:HH21  | 1.58                     | 0.68              |
| 13:N:31:GLU:HG2  | 13:N:33:LEU:H     | 1.59                     | 0.68              |
| 1:2:125:C:OP2    | 8:I:198:ARG:NH2   | 2.26                     | 0.68              |
| 37:z:575:A:H8    | 37:z:576:C:H4'    | 1.59                     | 0.68              |
| 1:2:868:A:HO2'   | 1:2:869:G:H8      | 1.38                     | 0.68              |
| 1:2:1394:G:H1    | 1:2:1444:A:N6     | 1.89                     | 0.68              |
| 13:N:97:ARG:O    | 13:N:97:ARG:NH1   | 2.24                     | 0.68              |
| 3:D:51:ARG:O     | 3:D:53:GLN:NE2    | 2.27                     | 0.68              |
| 6:G:31:PRO:HG3   | 6:G:43:PRO:HG3    | 1.76                     | 0.68              |
| 1:2:409:G:O3'    | 24:Y:88:LYS:NZ    | 2.26                     | 0.67              |
| 1:2:1204:A:OP1   | 1:2:1831:G:N2     | 2.27                     | 0.67              |
| 1:2:1123:C:O2'   | 28:c:17:ARG:NH1   | 2.27                     | 0.67              |
| 37:z:589:C:H2'   | 37:z:590:A:C8     | 2.28                     | 0.67              |
| 1:2:980:C:O2'    | 16:Q:138:ASP:O    | 2.12                     | 0.67              |
| 1:2:876:G:H2'    | 1:2:877:G:H8      | 1.58                     | 0.67              |
| 1:2:1584:A:H5''  | 21:V:82:ARG:HD2   | 1.76                     | 0.67              |
| 2:C:80:ARG:HE    | 2:C:81:ASN:H      | 1.41                     | 0.67              |
| 18:S:11:GLN:HG2  | 18:S:24:HIS:HB3   | 1.76                     | 0.67              |
| 32:g:87:LEU:HB2  | 32:g:101:PHE:HB2  | 1.75                     | 0.67              |
| 1:2:1588:C:OP2   | 33:h:104:ARG:NH1  | 2.27                     | 0.67              |
| 18:S:58:LEU:HG   | 18:S:108:ILE:HD11 | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:492:C:N3      | 26:a:84:LYS:NZ    | 2.43                     | 0.67              |
| 1:2:1279:C:H42    | 14:O:102:LYS:HA   | 1.60                     | 0.67              |
| 1:2:1517:A:O2'    | 20:U:144:ARG:NH1  | 2.26                     | 0.67              |
| 1:2:1598:G:N7     | 20:U:24:ARG:NH1   | 2.41                     | 0.67              |
| 24:Y:55:ASP:OD2   | 24:Y:60:LYS:NZ    | 2.28                     | 0.67              |
| 15:P:56:ASP:OD1   | 28:c:52:THR:OG1   | 2.12                     | 0.67              |
| 1:2:1643:G:N2     | 1:2:1670:A:OP2    | 2.27                     | 0.67              |
| 5:F:95:GLY:HA2    | 5:F:126:ILE:HG22  | 1.76                     | 0.67              |
| 17:R:10:ARG:NH1   | 17:R:10:ARG:O     | 2.27                     | 0.67              |
| 26:a:7:ILE:HG23   | 26:a:25:ILE:HD11  | 1.77                     | 0.67              |
| 32:g:283:PRO:O    | 32:g:285:GLN:NE2  | 2.27                     | 0.67              |
| 11:L:134:HIS:CE1  | 11:L:164:PRO:HD2  | 2.30                     | 0.67              |
| 18:S:138:ARG:NH1  | 18:S:138:ARG:O    | 2.27                     | 0.67              |
| 34:i:118:ASN:H    | 34:i:119:VAL:HA   | 1.60                     | 0.67              |
| 1:2:67:C:N4       | 1:2:151:C:O2'     | 2.28                     | 0.66              |
| 1:2:1534:U:H2'    | 1:2:1535:G:H8     | 1.60                     | 0.66              |
| 33:h:106:GLN:NE2  | 33:h:107:VAL:O    | 2.27                     | 0.66              |
| 3:D:179:ASN:HB3   | 3:D:183:GLU:HB3   | 1.76                     | 0.66              |
| 20:U:30:ILE:HG22  | 20:U:36:VAL:HG11  | 1.78                     | 0.66              |
| 5:F:137:VAL:HB    | 5:F:185:LYS:HB3   | 1.77                     | 0.66              |
| 1:2:922:A:H61     | 1:2:1011:U:H5     | 1.44                     | 0.66              |
| 1:2:1688:G:H21    | 1:2:1828:A:H8     | 1.43                     | 0.66              |
| 15:P:11:LEU:HD21  | 28:c:21:LYS:HD2   | 1.77                     | 0.66              |
| 26:a:15:ASN:HD21  | 26:a:18:LEU:HD12  | 1.59                     | 0.66              |
| 26:a:106:GLN:N    | 26:a:106:GLN:OE1  | 2.29                     | 0.66              |
| 1:2:1309:A:OP2    | 14:O:33:ARG:NH2   | 2.29                     | 0.66              |
| 2:C:89:LYS:HE2    | 2:C:201:LEU:HG    | 1.78                     | 0.66              |
| 1:2:965:U:H3'     | 1:2:966:G:H21     | 1.61                     | 0.66              |
| 27:b:22:ARG:NH1   | 27:b:29:CYS:SG    | 2.69                     | 0.66              |
| 1:2:1755:U:O2     | 1:2:1765:G:N2     | 2.29                     | 0.66              |
| 1:2:886:U:H5'     | 1:2:887:G:H5''    | 1.78                     | 0.65              |
| 33:h:57:LYS:HE3   | 33:h:61:GLU:HB3   | 1.78                     | 0.65              |
| 1:2:189:G:H1'     | 1:2:206:A:N6      | 2.11                     | 0.65              |
| 1:2:937:C:H2'     | 1:2:938:G:H8      | 1.60                     | 0.65              |
| 10:K:37:LYS:NZ    | 10:K:93:THR:O     | 2.29                     | 0.65              |
| 16:Q:142:ARG:HH21 | 27:b:22:ARG:HB3   | 1.61                     | 0.65              |
| 32:g:220:ASP:HB2  | 32:g:227:LEU:HD21 | 1.79                     | 0.65              |
| 1:2:667:G:N1      | 1:2:1023:A:OP2    | 2.26                     | 0.65              |
| 1:2:1199:G:H4'    | 4:E:101:THR:HA    | 1.78                     | 0.65              |
| 1:2:745:U:H2'     | 1:2:746:C:C6      | 2.32                     | 0.65              |
| 1:2:1712:C:O2'    | 35:l:21:ARG:NH2   | 2.28                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 19:T:18:GLU:HG3  | 19:T:69:ILE:HD12  | 1.77                     | 0.65              |
| 1:2:427:G:H3'    | 1:2:428:G:H21     | 1.61                     | 0.65              |
| 1:2:1099:C:H2'   | 1:2:1100:G:C8     | 2.31                     | 0.65              |
| 2:C:141:ASN:HD21 | 23:X:29:HIS:HA    | 1.61                     | 0.65              |
| 6:G:43:PRO:HD2   | 6:G:46:ILE:HD12   | 1.78                     | 0.65              |
| 20:U:147:GLY:HA2 | 36:y:27:U:H5''    | 1.78                     | 0.65              |
| 21:V:33:TRP:HZ2  | 21:V:102:ARG:HG3  | 1.62                     | 0.65              |
| 1:2:192:U:OP2    | 10:K:143:LYS:NZ   | 2.29                     | 0.65              |
| 1:2:1223:G:H1    | 1:2:1526:A:N6     | 1.95                     | 0.65              |
| 2:C:163:CYS:SG   | 2:C:164:ASN:N     | 2.70                     | 0.65              |
| 17:R:111:MET:HE1 | 20:U:117:ILE:HG23 | 1.79                     | 0.65              |
| 24:Y:7:LEU:HD11  | 24:Y:37:PHE:HD2   | 1.59                     | 0.65              |
| 1:2:1152:U:O4    | 4:E:179:ARG:NH1   | 2.30                     | 0.65              |
| 1:2:1350:G:N2    | 1:2:1353:A:OP2    | 2.27                     | 0.65              |
| 1:2:1709:U:H2'   | 1:2:1710:A:H8     | 1.62                     | 0.65              |
| 1:2:835:C:H1'    | 1:2:837:G:H1'     | 1.77                     | 0.64              |
| 8:I:42:GLY:O     | 8:I:46:LYS:NZ     | 2.29                     | 0.64              |
| 1:2:487:C:H4'    | 6:G:8:HIS:HD2     | 1.62                     | 0.64              |
| 1:2:903:G:H2'    | 1:2:904:A:C8      | 2.32                     | 0.64              |
| 1:2:1211:C:H42   | 1:2:1216:A:H61    | 1.45                     | 0.64              |
| 1:2:1382:A:OP2   | 5:F:160:SER:OG    | 2.14                     | 0.64              |
| 1:2:1802:U:H2'   | 1:2:1803:A:C8     | 2.31                     | 0.64              |
| 9:J:139:ILE:O    | 15:P:19:ARG:NH2   | 2.28                     | 0.64              |
| 32:g:159:ASN:ND2 | 32:g:162:ASN:O    | 2.30                     | 0.64              |
| 1:2:1588:C:O2'   | 18:S:45:ARG:NH2   | 2.30                     | 0.64              |
| 21:V:125:PRO:O   | 21:V:128:GLN:NE2  | 2.29                     | 0.64              |
| 1:2:599:U:H2'    | 1:2:600:G:C8      | 2.33                     | 0.64              |
| 1:2:941:U:H2'    | 1:2:942:U:C6      | 2.32                     | 0.64              |
| 4:E:45:TRP:NE1   | 4:E:77:GLU:OE2    | 2.30                     | 0.64              |
| 1:2:915:A:OP1    | 24:Y:57:ARG:NH1   | 2.30                     | 0.64              |
| 1:2:1493:G:N7    | 12:M:25:LYS:NZ    | 2.45                     | 0.64              |
| 15:P:19:ARG:HH11 | 15:P:21:SER:HB2   | 1.62                     | 0.64              |
| 1:2:2:A:H5'      | 1:2:408:A:H5'     | 1.79                     | 0.64              |
| 1:2:537:G:H2'    | 1:2:538:C:C6      | 2.33                     | 0.64              |
| 1:2:1773:G:H2'   | 1:2:1774:G:C8     | 2.33                     | 0.64              |
| 18:S:128:GLU:OE2 | 18:S:128:GLU:N    | 2.29                     | 0.64              |
| 1:2:295:C:O2     | 10:K:184:ARG:NH2  | 2.31                     | 0.64              |
| 7:H:156:THR:HA   | 7:H:159:ARG:HH21  | 1.63                     | 0.64              |
| 12:M:61:GLN:HB2  | 12:M:68:TYR:HB2   | 1.78                     | 0.64              |
| 13:N:103:GLU:OE2 | 25:Z:11:ARG:NH1   | 2.31                     | 0.64              |
| 23:X:71:ARG:HH22 | 24:Y:23:ARG:HH11  | 1.45                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:106:C:H2'    | 1:2:107:A:H8      | 1.63                     | 0.64              |
| 1:2:923:C:O2     | 28:c:51:GLN:NE2   | 2.31                     | 0.64              |
| 3:D:80:ALA:O     | 3:D:83:LYS:NZ     | 2.31                     | 0.64              |
| 3:D:107:ARG:NH2  | 16:Q:131:ASP:OD2  | 2.30                     | 0.64              |
| 7:H:71:ARG:NH2   | 7:H:148:ASN:OD1   | 2.31                     | 0.64              |
| 32:g:13:GLY:HA3  | 32:g:43:TRP:HH2   | 1.62                     | 0.64              |
| 15:P:99:ARG:NH1  | 15:P:141:TYR:OH   | 2.31                     | 0.64              |
| 22:W:82:MET:HE1  | 30:e:52:PHE:HA    | 1.78                     | 0.64              |
| 1:2:635:C:H2'    | 1:2:636:G:H8      | 1.63                     | 0.64              |
| 1:2:202:U:H2'    | 1:2:203:G:C8      | 2.32                     | 0.63              |
| 6:G:141:THR:OG1  | 6:G:143:ASP:OD1   | 2.13                     | 0.63              |
| 10:K:72:CYS:HG   | 10:K:112:TRP:CD1  | 2.16                     | 0.63              |
| 4:E:79:ILE:HG12  | 4:E:147:ILE:HD12  | 1.80                     | 0.63              |
| 6:G:175:PHE:O    | 6:G:198:ARG:NH2   | 2.26                     | 0.63              |
| 17:R:34:MET:SD   | 17:R:35:GLN:NE2   | 2.71                     | 0.63              |
| 30:e:22:ARG:HH21 | 30:e:37:ASN:H     | 1.47                     | 0.63              |
| 1:2:55:U:OP1     | 1:2:441:G:N1      | 2.31                     | 0.63              |
| 1:2:1534:U:H2'   | 1:2:1535:G:C8     | 2.33                     | 0.63              |
| 3:D:22:VAL:O     | 3:D:27:LYS:NZ     | 2.31                     | 0.63              |
| 8:I:63:MET:HE1   | 8:I:98:ARG:HB3    | 1.80                     | 0.63              |
| 17:R:15:PHE:HB3  | 20:U:91:LYS:HD3   | 1.79                     | 0.63              |
| 18:S:146:ARG:NH2 | 36:y:32:C:OP2     | 2.30                     | 0.63              |
| 1:2:1440:U:OP1   | 18:S:15:ARG:NH2   | 2.32                     | 0.63              |
| 2:C:85:ARG:NH1   | 2:C:201:LEU:O     | 2.31                     | 0.63              |
| 3:D:30:TRP:HB2   | 16:Q:20:GLN:HE22  | 1.62                     | 0.63              |
| 10:K:48:VAL:HG22 | 10:K:49:ARG:H     | 1.62                     | 0.63              |
| 1:2:492:C:O3'    | 6:G:62:LYS:NZ     | 2.29                     | 0.63              |
| 1:2:821:A:H2'    | 1:2:822:A:H8      | 1.64                     | 0.63              |
| 1:2:1007:A:H5''  | 15:P:3:ARG:HH22   | 1.64                     | 0.63              |
| 14:O:35:ILE:HG13 | 31:f:103:LEU:HD13 | 1.81                     | 0.63              |
| 19:T:103:LYS:O   | 19:T:107:LYS:N    | 2.31                     | 0.63              |
| 1:2:1138:G:N2    | 1:2:1141:A:OP2    | 2.30                     | 0.63              |
| 31:f:139:HIS:HB2 | 31:f:150:PHE:HB2  | 1.80                     | 0.63              |
| 1:2:815:G:OP2    | 11:L:80:ARG:NH1   | 2.32                     | 0.63              |
| 1:2:1588:C:OP1   | 7:H:91:ARG:NE     | 2.31                     | 0.63              |
| 1:2:75:G:OP2     | 1:2:75:G:N2       | 2.27                     | 0.62              |
| 1:2:168:C:O2'    | 8:I:133:LEU:O     | 2.16                     | 0.62              |
| 37:z:551:C:H2'   | 37:z:552:A:C8     | 2.33                     | 0.62              |
| 1:2:155:G:H2'    | 1:2:156:G:H8      | 1.64                     | 0.62              |
| 1:2:550:A:OP2    | 11:L:177:ASN:ND2  | 2.31                     | 0.62              |
| 1:2:978:G:H2'    | 1:2:979:A:H8      | 1.64                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 37:z:595:C:H2'   | 37:z:596:A:H8    | 1.64                     | 0.62              |
| 1:2:671:U:H4'    | 25:Z:9:THR:HG22  | 1.81                     | 0.62              |
| 8:I:1:MET:N      | 8:I:18:VAL:O     | 2.31                     | 0.62              |
| 13:N:7:GLU:HG2   | 13:N:9:ALA:H     | 1.63                     | 0.62              |
| 32:g:34:ALA:HA   | 32:g:40:ILE:HG22 | 1.82                     | 0.62              |
| 1:2:42:A:O2'     | 1:2:98:C:OP1     | 2.14                     | 0.62              |
| 1:2:148:U:H2'    | 1:2:149:A:H8     | 1.63                     | 0.62              |
| 1:2:940:A:N6     | 1:2:978:G:H1     | 1.96                     | 0.62              |
| 1:2:1043:C:H5''  | 16:Q:143:LYS:HD3 | 1.82                     | 0.62              |
| 1:2:483:A:H62    | 1:2:499:G:H21    | 1.47                     | 0.62              |
| 1:2:1612:G:N7    | 17:R:43:ARG:NH2  | 2.46                     | 0.62              |
| 4:E:106:ARG:HH12 | 4:E:108:ARG:HE   | 1.47                     | 0.62              |
| 13:N:80:MET:SD   | 13:N:86:ILE:HG13 | 2.40                     | 0.62              |
| 36:y:27:U:H2'    | 36:y:28:G:H8     | 1.64                     | 0.62              |
| 1:2:487:C:H4'    | 6:G:8:HIS:CD2    | 2.34                     | 0.62              |
| 1:2:1216:A:N3    | 1:2:1672:U:O2'   | 2.27                     | 0.62              |
| 1:2:1409:G:H2'   | 1:2:1410:A:H8    | 1.64                     | 0.62              |
| 32:g:32:LEU:HD21 | 32:g:92:LEU:HD21 | 1.80                     | 0.62              |
| 1:2:1086:C:H2'   | 1:2:1087:C:C6    | 2.34                     | 0.62              |
| 13:N:60:CYS:SG   | 13:N:63:THR:OG1  | 2.55                     | 0.62              |
| 18:S:23:ALA:HB1  | 18:S:68:ILE:HD11 | 1.82                     | 0.62              |
| 1:2:832:G:N2     | 1:2:834:G:OP2    | 2.33                     | 0.62              |
| 1:2:1331:G:H1    | 1:2:1488:U:H3    | 1.48                     | 0.62              |
| 2:C:124:VAL:HG11 | 2:C:134:LEU:HD21 | 1.81                     | 0.62              |
| 3:D:164:ILE:O    | 3:D:168:MET:HG2  | 2.00                     | 0.62              |
| 1:2:1161:G:OP2   | 1:2:1161:G:N2    | 2.24                     | 0.62              |
| 1:2:1224:A:H2'   | 1:2:1225:G:C8    | 2.35                     | 0.62              |
| 1:2:1276:G:H22   | 1:2:1313:U:H3    | 1.45                     | 0.62              |
| 4:E:218:LEU:HA   | 4:E:221:PHE:HB2  | 1.82                     | 0.62              |
| 7:H:168:THR:OG1  | 7:H:171:GLU:OE1  | 2.16                     | 0.62              |
| 1:2:124:U:OP1    | 6:G:148:ARG:NH2  | 2.33                     | 0.61              |
| 1:2:628:C:H2'    | 1:2:629:C:H6     | 1.65                     | 0.61              |
| 1:2:909:A:N6     | 9:J:120:ARG:HA   | 2.14                     | 0.61              |
| 2:C:7:VAL:HG11   | 23:X:43:THR:HA   | 1.82                     | 0.61              |
| 32:g:238:ALA:H   | 32:g:251:ALA:HB3 | 1.65                     | 0.61              |
| 1:2:307:G:H3'    | 8:I:183:ARG:HH22 | 1.64                     | 0.61              |
| 1:2:1134:C:OP1   | 2:C:155:ARG:NH1  | 2.33                     | 0.61              |
| 2:C:74:VAL:HG22  | 2:C:121:LEU:HB2  | 1.82                     | 0.61              |
| 25:Z:134:TYR:OH  | 34:i:87:ARG:NH2  | 2.33                     | 0.61              |
| 36:y:9:G:N1      | 36:y:15:G:O6     | 2.33                     | 0.61              |
| 1:2:1659:A:O2'   | 1:2:1660:G:H5'   | 2.01                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1845:A:OP1    | 35:l:9:ARG:NH2    | 2.33                     | 0.61              |
| 2:C:121:LEU:HD13  | 2:C:143:PRO:HG2   | 1.81                     | 0.61              |
| 1:2:1344:G:H22    | 1:2:1377:G:H1     | 1.47                     | 0.61              |
| 1:2:1611:U:O2'    | 1:2:1656:A:O2'    | 2.16                     | 0.61              |
| 2:C:17:LYS:HE2    | 2:C:176:TRP:HZ3   | 1.64                     | 0.61              |
| 37:z:595:C:H2'    | 37:z:596:A:C8     | 2.35                     | 0.61              |
| 4:E:162:PRO:HG2   | 23:X:9:VAL:HG21   | 1.81                     | 0.61              |
| 10:K:199:LEU:HD13 | 10:K:202:ILE:HD11 | 1.81                     | 0.61              |
| 17:R:8:LYS:O      | 17:R:14:LYS:HB3   | 2.00                     | 0.61              |
| 24:Y:71:LYS:N     | 24:Y:130:PHE:O    | 2.33                     | 0.61              |
| 1:2:162:C:O2'     | 8:I:95:LYS:NZ     | 2.34                     | 0.61              |
| 1:2:1361:G:H2'    | 1:2:1362:G:C8     | 2.36                     | 0.61              |
| 1:2:1643:G:H5''   | 18:S:125:ARG:HG3  | 1.81                     | 0.61              |
| 8:I:130:PRO:O     | 8:I:132:ARG:NH1   | 2.33                     | 0.61              |
| 29:d:13:ARG:HA    | 29:d:55:VAL:HA    | 1.80                     | 0.61              |
| 1:2:72:C:O4'      | 1:2:74:G:N2       | 2.34                     | 0.61              |
| 16:Q:33:ILE:N     | 16:Q:96:LYS:O     | 2.32                     | 0.61              |
| 26:a:16:ARG:O     | 26:a:19:GLN:NE2   | 2.33                     | 0.61              |
| 4:E:161:LYS:O     | 4:E:185:ARG:NH2   | 2.34                     | 0.61              |
| 13:N:40:ILE:HG23  | 13:N:68:ILE:HD13  | 1.83                     | 0.61              |
| 4:E:63:LEU:HG     | 4:E:82:PHE:HD1    | 1.65                     | 0.61              |
| 29:d:27:CYS:SG    | 29:d:28:THR:N     | 2.74                     | 0.61              |
| 1:2:1586:C:OP1    | 7:H:85:LYS:NZ     | 2.28                     | 0.61              |
| 1:2:1802:U:H2'    | 1:2:1803:A:H8     | 1.66                     | 0.61              |
| 17:R:86:LEU:H     | 17:R:89:MET:HE2   | 1.66                     | 0.61              |
| 32:g:88:ARG:HD3   | 32:g:97:THR:HG21  | 1.81                     | 0.61              |
| 1:2:978:G:H2'     | 1:2:979:A:C8      | 2.35                     | 0.60              |
| 1:2:1232:G:H21    | 1:2:1517:A:N6     | 1.98                     | 0.60              |
| 1:2:1792:C:HO2'   | 10:K:2:GLY:N      | 1.98                     | 0.60              |
| 10:K:64:ASN:HA    | 10:K:75:LYS:HA    | 1.83                     | 0.60              |
| 10:K:144:LYS:N    | 10:K:147:LYS:HE2  | 2.14                     | 0.60              |
| 24:Y:41:MET:HB3   | 24:Y:47:ILE:HD12  | 1.83                     | 0.60              |
| 1:2:434:G:H1      | 10:K:26:LYS:HE3   | 1.66                     | 0.60              |
| 1:2:882:A:H61     | 1:2:896:C:H42     | 1.48                     | 0.60              |
| 1:2:1394:G:N2     | 1:2:1444:A:N1     | 2.45                     | 0.60              |
| 1:2:1716:U:H4'    | 1:2:1717:G:H5''   | 1.83                     | 0.60              |
| 5:F:214:LYS:HD3   | 19:T:19:LYS:HB3   | 1.84                     | 0.60              |
| 6:G:128:LYS:H     | 6:G:140:VAL:HB    | 1.66                     | 0.60              |
| 16:Q:142:ARG:HE   | 27:b:22:ARG:HB3   | 1.66                     | 0.60              |
| 17:R:60:LEU:HD13  | 17:R:89:MET:HG3   | 1.83                     | 0.60              |
| 18:S:130:LYS:HA   | 18:S:137:ALA:HA   | 1.82                     | 0.60              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 24:Y:46:TYR:HA    | 24:Y:68:ARG:HG2  | 1.83                     | 0.60              |
| 32:g:122:SER:OG   | 32:g:132:TRP:NE1 | 2.33                     | 0.60              |
| 36:y:54:U:N3      | 36:y:57:A:OP2    | 2.34                     | 0.60              |
| 1:2:1441:U:H4'    | 22:W:57:PRO:HG3  | 1.82                     | 0.60              |
| 1:2:1574:A:O2'    | 1:2:1576:C:OP2   | 2.14                     | 0.60              |
| 3:D:46:LYS:HE3    | 16:Q:27:VAL:HB   | 1.82                     | 0.60              |
| 6:G:153:LEU:HD13  | 8:I:216:ARG:HH22 | 1.65                     | 0.60              |
| 1:2:165:G:H2'     | 1:2:166:A:C8     | 2.36                     | 0.60              |
| 1:2:378:U:H2'     | 1:2:379:A:H8     | 1.66                     | 0.60              |
| 1:2:1123:C:H4'    | 28:c:17:ARG:HH12 | 1.67                     | 0.60              |
| 1:2:1815:U:H2'    | 1:2:1816:A:H8    | 1.66                     | 0.60              |
| 13:N:16:ILE:HG13  | 13:N:17:PHE:H    | 1.66                     | 0.60              |
| 1:2:431:C:H2'     | 1:2:432:C:C6     | 2.37                     | 0.60              |
| 1:2:1108:U:H3     | 1:2:1109:A:N6    | 2.00                     | 0.60              |
| 2:C:113:GLN:HB2   | 2:C:116:PHE:HB2  | 1.84                     | 0.60              |
| 8:I:74:ARG:NH1    | 8:I:96:SER:OG    | 2.34                     | 0.60              |
| 12:M:1:MET:H2     | 12:M:2:LEU:HB3   | 1.66                     | 0.60              |
| 24:Y:102:ILE:HG12 | 24:Y:113:HIS:HD2 | 1.67                     | 0.60              |
| 1:2:9:U:N3        | 1:2:12:U:OP2     | 2.33                     | 0.60              |
| 1:2:480:C:O2'     | 1:2:564:A:N1     | 2.35                     | 0.60              |
| 1:2:1273:C:H2'    | 1:2:1274:A:H8    | 1.67                     | 0.60              |
| 7:H:34:SER:HA     | 29:d:55:VAL:HG13 | 1.82                     | 0.60              |
| 12:M:65:ARG:NH2   | 30:e:21:CYS:O    | 2.35                     | 0.60              |
| 16:Q:29:GLY:O     | 16:Q:94:HIS:N    | 2.31                     | 0.60              |
| 23:X:14:PRO:HB2   | 23:X:23:ILE:HD11 | 1.82                     | 0.60              |
| 1:2:145:G:H2'     | 1:2:146:G:C8     | 2.36                     | 0.60              |
| 1:2:911:G:N2      | 1:2:911:G:OP2    | 2.35                     | 0.60              |
| 1:2:1281:G:N1     | 31:f:103:LEU:O   | 2.35                     | 0.60              |
| 32:g:209:SER:HG   | 32:g:219:TRP:CD1 | 2.20                     | 0.60              |
| 36:y:26:C:H2'     | 36:y:27:U:C6     | 2.37                     | 0.60              |
| 9:J:145:ARG:NH2   | 24:Y:49:GLU:HG3  | 2.17                     | 0.60              |
| 1:2:483:A:N6      | 1:2:500:G:H1'    | 2.15                     | 0.60              |
| 1:2:1388:U:H2'    | 1:2:1389:G:C8    | 2.36                     | 0.60              |
| 1:2:1541:G:H22    | 1:2:1650:C:H1'   | 1.67                     | 0.60              |
| 1:2:220:C:H2'     | 1:2:221:A:C8     | 2.36                     | 0.59              |
| 1:2:971:G:OP1     | 16:Q:98:ARG:NH1  | 2.35                     | 0.59              |
| 1:2:1643:G:C8     | 18:S:125:ARG:HG2 | 2.37                     | 0.59              |
| 9:J:46:THR:HB     | 9:J:65:PRO:HG3   | 1.82                     | 0.59              |
| 21:V:104:LEU:HD22 | 21:V:121:ARG:HG2 | 1.82                     | 0.59              |
| 22:W:70:CYS:H     | 30:e:40:ARG:HH22 | 1.50                     | 0.59              |
| 1:2:1612:G:H1     | 17:R:40:ARG:HH22 | 1.50                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:E:115:ILE:O    | 4:E:123:GLY:N    | 2.34                     | 0.59              |
| 7:H:28:VAL:HA    | 7:H:110:GLN:HG3  | 1.84                     | 0.59              |
| 7:H:198:ARG:HA   | 7:H:201:LYS:HG2  | 1.84                     | 0.59              |
| 20:U:61:GLU:N    | 20:U:61:GLU:OE2  | 2.35                     | 0.59              |
| 1:2:403:G:OP1    | 1:2:809:A:N6     | 2.36                     | 0.59              |
| 1:2:1631:G:N7    | 33:h:41:ARG:NH1  | 2.49                     | 0.59              |
| 8:I:51:ARG:NH1   | 8:I:52:ILE:O     | 2.36                     | 0.59              |
| 9:J:129:ILE:HD11 | 9:J:180:LEU:HD13 | 1.85                     | 0.59              |
| 1:2:349:U:H5'    | 25:Z:22:TRP:HH2  | 1.68                     | 0.59              |
| 1:2:1091:U:O3'   | 24:Y:20:ARG:NH1  | 2.32                     | 0.59              |
| 1:2:1117:G:O2'   | 3:D:204:ILE:O    | 2.20                     | 0.59              |
| 7:H:145:ARG:HA   | 7:H:148:ASN:HD22 | 1.67                     | 0.59              |
| 18:S:70:VAL:HG11 | 18:S:84:ILE:HG22 | 1.83                     | 0.59              |
| 1:2:492:C:O2     | 6:G:63:LYS:NZ    | 2.36                     | 0.59              |
| 1:2:1376:C:H2'   | 1:2:1377:G:C8    | 2.36                     | 0.59              |
| 3:D:103:MET:HG3  | 3:D:215:VAL:HB   | 1.84                     | 0.59              |
| 7:H:126:THR:OG1  | 29:d:26:GLN:OE1  | 2.15                     | 0.59              |
| 1:2:110:U:O2'    | 13:N:71:ARG:NH1  | 2.35                     | 0.59              |
| 10:K:23:LYS:O    | 10:K:25:ARG:NH1  | 2.35                     | 0.59              |
| 37:z:552:A:H2'   | 37:z:553:G:C8    | 2.38                     | 0.59              |
| 1:2:378:U:H2'    | 1:2:379:A:C8     | 2.38                     | 0.59              |
| 4:E:241:TRP:CG   | 24:Y:68:ARG:HE   | 2.20                     | 0.59              |
| 6:G:10:LYS:HZ2   | 6:G:12:VAL:HB    | 1.67                     | 0.59              |
| 1:2:866:A:N6     | 1:2:912:A:O5'    | 2.35                     | 0.59              |
| 1:2:1282:G:N2    | 1:2:1308:G:O2'   | 2.34                     | 0.59              |
| 1:2:1859:C:OP2   | 27:b:92:ARG:NH1  | 2.36                     | 0.59              |
| 13:N:87:VAL:HA   | 13:N:110:SER:HA  | 1.85                     | 0.59              |
| 14:O:13:ASP:HB3  | 14:O:16:THR:HG22 | 1.84                     | 0.59              |
| 15:P:119:GLU:OE2 | 15:P:123:HIS:NE2 | 2.36                     | 0.59              |
| 17:R:123:TYR:OH  | 20:U:124:ARG:NH1 | 2.35                     | 0.59              |
| 1:2:841:G:H2'    | 1:2:842:G:C8     | 2.38                     | 0.59              |
| 1:2:920:G:N2     | 15:P:87:ASP:OD2  | 2.35                     | 0.59              |
| 1:2:1276:G:H1    | 1:2:1313:U:H3    | 1.51                     | 0.59              |
| 26:a:24:VAL:HA   | 26:a:72:PHE:HA   | 1.83                     | 0.59              |
| 1:2:1687:U:H2'   | 1:2:1688:G:C8    | 2.38                     | 0.59              |
| 5:F:6:SER:O      | 5:F:10:LYS:N     | 2.36                     | 0.59              |
| 5:F:22:ASN:OD1   | 5:F:23:GLU:N     | 2.36                     | 0.59              |
| 36:y:24:U:H2'    | 36:y:25:G:H8     | 1.68                     | 0.59              |
| 1:2:308:C:OP2    | 8:I:183:ARG:NH2  | 2.35                     | 0.58              |
| 1:2:741:C:H42    | 1:2:793:C:H42    | 1.51                     | 0.58              |
| 1:2:1245:C:H5''  | 1:2:1246:A:H2'   | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1249:A:O2'    | 1:2:1661:C:O2'    | 2.18                     | 0.58              |
| 1:2:1601:G:OP1    | 21:V:84:ARG:NH2   | 2.36                     | 0.58              |
| 1:2:1751:G:O6     | 1:2:1769:U:O4     | 2.21                     | 0.58              |
| 6:G:71:LYS:HB2    | 6:G:91:SER:HB2    | 1.85                     | 0.58              |
| 37:z:522:U:H2'    | 37:z:523:G:H8     | 1.67                     | 0.58              |
| 1:2:511:A:OP1     | 11:L:45:ARG:NH1   | 2.37                     | 0.58              |
| 1:2:633:A:OP2     | 11:L:38:ARG:NH1   | 2.35                     | 0.58              |
| 1:2:1560:C:H2'    | 1:2:1561:G:C8     | 2.38                     | 0.58              |
| 3:D:60:ASP:HA     | 3:D:63:LYS:HD2    | 1.84                     | 0.58              |
| 7:H:195:GLU:HA    | 7:H:198:ARG:HB2   | 1.83                     | 0.58              |
| 17:R:32:GLN:OE1   | 17:R:32:GLN:N     | 2.35                     | 0.58              |
| 20:U:115:LYS:NZ   | 37:z:566:C:OP1    | 2.35                     | 0.58              |
| 31:f:123:SER:HG   | 31:f:144:CYS:HG   | 1.51                     | 0.58              |
| 37:z:532:G:O6     | 37:z:559:U:N3     | 2.36                     | 0.58              |
| 1:2:166:A:H2'     | 1:2:167:G:H8      | 1.68                     | 0.58              |
| 1:2:1139:A:H2'    | 1:2:1140:A:C8     | 2.38                     | 0.58              |
| 1:2:1724:U:O2     | 1:2:1799:G:N2     | 2.33                     | 0.58              |
| 1:2:1825:A:O2'    | 1:2:1846:C:OP1    | 2.20                     | 0.58              |
| 10:K:162:LEU:HB3  | 10:K:166:PHE:HE2  | 1.68                     | 0.58              |
| 15:P:85:PRO:HD2   | 15:P:88:LEU:HD12  | 1.85                     | 0.58              |
| 1:2:1294:G:OP2    | 17:R:77:LYS:NZ    | 2.36                     | 0.58              |
| 1:2:1450:A:OP1    | 19:T:3:ARG:NH1    | 2.37                     | 0.58              |
| 4:E:69:PHE:HD2    | 4:E:71:LEU:HB2    | 1.68                     | 0.58              |
| 23:X:31:SER:OG    | 23:X:57:GLY:N     | 2.36                     | 0.58              |
| 33:h:106:GLN:HE22 | 33:h:108:ILE:HD13 | 1.67                     | 0.58              |
| 1:2:158:A:H2'     | 1:2:159:A:C8      | 2.38                     | 0.58              |
| 3:D:40:ASN:H      | 3:D:75:GLN:HE22   | 1.51                     | 0.58              |
| 36:y:18:G:H21     | 36:y:19:A:H61     | 1.51                     | 0.58              |
| 37:z:547:G:N1     | 37:z:550:A:OP2    | 2.34                     | 0.58              |
| 1:2:65:C:N4       | 1:2:169:U:O2'     | 2.37                     | 0.58              |
| 1:2:538:C:H2'     | 1:2:539:C:C6      | 2.38                     | 0.58              |
| 1:2:678:U:H3      | 9:J:102:PRO:HA    | 1.67                     | 0.58              |
| 1:2:784:G:H4'     | 8:I:237:LEU:HB2   | 1.85                     | 0.58              |
| 19:T:20:TYR:CZ    | 19:T:38:ILE:HD11  | 2.39                     | 0.58              |
| 29:d:20:ARG:NH2   | 29:d:25:GLY:O     | 2.37                     | 0.58              |
| 32:g:131:LEU:N    | 32:g:140:TYR:O    | 2.36                     | 0.58              |
| 1:2:127:C:O2'     | 1:2:212:G:OP2     | 2.20                     | 0.58              |
| 1:2:166:A:H2'     | 1:2:167:G:C8      | 2.39                     | 0.58              |
| 1:2:431:C:H4'     | 1:2:1733:C:H5'    | 1.84                     | 0.58              |
| 1:2:874:G:O6      | 1:2:904:A:N1      | 2.36                     | 0.58              |
| 1:2:970:C:H2'     | 1:2:971:G:H8      | 1.69                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:1188:U:H2'   | 1:2:1189:U:C6     | 2.39                     | 0.58              |
| 2:C:36:GLN:OE1   | 2:C:36:GLN:N      | 2.31                     | 0.58              |
| 10:K:191:GLU:OE1 | 13:N:20:LYS:NZ    | 2.32                     | 0.58              |
| 28:c:34:ASP:HB3  | 28:c:80:ARG:HG3   | 1.85                     | 0.58              |
| 36:y:9:G:N2      | 36:y:20:A:O4'     | 2.36                     | 0.58              |
| 1:2:52:G:O2'     | 26:a:105:LYS:NZ   | 2.37                     | 0.58              |
| 1:2:376:C:H1'    | 10:K:5:ARG:HG3    | 1.86                     | 0.58              |
| 1:2:384:G:H2'    | 1:2:385:G:H8      | 1.68                     | 0.58              |
| 1:2:1006:G:H2'   | 1:2:1007:A:H8     | 1.69                     | 0.58              |
| 1:2:1611:U:H3    | 1:2:1615:A:H62    | 1.50                     | 0.58              |
| 2:C:33:GLN:NE2   | 23:X:64:GLU:OE2   | 2.37                     | 0.58              |
| 7:H:144:LEU:O    | 7:H:148:ASN:ND2   | 2.37                     | 0.58              |
| 22:W:23:THR:HA   | 22:W:88:LEU:HA    | 1.86                     | 0.58              |
| 24:Y:90:GLN:HB2  | 24:Y:94:LEU:HD12  | 1.86                     | 0.58              |
| 32:g:123:GLY:HA3 | 32:g:151:VAL:HG11 | 1.85                     | 0.58              |
| 1:2:19:A:H5'     | 25:Z:107:ARG:HH11 | 1.69                     | 0.58              |
| 1:2:1279:C:H4'   | 31:f:99:LYS:NZ    | 2.19                     | 0.58              |
| 2:C:4:ALA:HB3    | 2:C:8:LEU:HB2     | 1.84                     | 0.58              |
| 2:C:176:TRP:CE3  | 2:C:199:PRO:HB3   | 2.38                     | 0.58              |
| 8:I:188:LYS:HG3  | 8:I:191:ARG:HH12  | 1.68                     | 0.58              |
| 17:R:10:ARG:CZ   | 17:R:17:TYR:HB3   | 2.33                     | 0.58              |
| 17:R:41:GLN:NE2  | 17:R:113:GLY:O    | 2.36                     | 0.58              |
| 1:2:148:U:H3     | 1:2:170:A:H62     | 1.50                     | 0.57              |
| 1:2:740:G:O2'    | 1:2:741:C:OP1     | 2.21                     | 0.57              |
| 1:2:1371:G:H2'   | 1:2:1372:A:C8     | 2.39                     | 0.57              |
| 1:2:1562:G:H21   | 1:2:1562:G:P      | 2.26                     | 0.57              |
| 6:G:181:CYS:HA   | 6:G:227:VAL:HA    | 1.84                     | 0.57              |
| 7:H:22:LYS:NZ    | 7:H:98:GLU:OE1    | 2.37                     | 0.57              |
| 8:I:52:ILE:HD11  | 8:I:109:LEU:HD12  | 1.85                     | 0.57              |
| 19:T:17:ILE:HD11 | 19:T:21:TYR:HD1   | 1.69                     | 0.57              |
| 1:2:1203:G:N2    | 1:2:1831:G:O2'    | 2.37                     | 0.57              |
| 1:2:1544:U:OP1   | 30:e:34:TYR:OH    | 2.21                     | 0.57              |
| 1:2:1669:G:H5''  | 7:H:86:LYS:HE3    | 1.86                     | 0.57              |
| 13:N:77:VAL:HB   | 13:N:124:ASP:H    | 1.69                     | 0.57              |
| 37:z:579:G:H2'   | 37:z:580:U:C6     | 2.40                     | 0.57              |
| 1:2:970:C:H2'    | 1:2:971:G:C8      | 2.38                     | 0.57              |
| 3:D:222:LYS:HG2  | 3:D:223:PHE:H     | 1.69                     | 0.57              |
| 9:J:78:ARG:NH1   | 9:J:81:ARG:HH11   | 2.01                     | 0.57              |
| 16:Q:31:CYS:HB2  | 16:Q:95:ILE:HA    | 1.86                     | 0.57              |
| 22:W:48:LEU:HD23 | 22:W:91:LEU:HD23  | 1.86                     | 0.57              |
| 27:b:38:LYS:HB3  | 27:b:71:LEU:HD11  | 1.85                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 36:y:21:G:H2'     | 36:y:22:C:C6     | 2.39                     | 0.57              |
| 1:2:520:U:H2'     | 1:2:521:A:C8     | 2.38                     | 0.57              |
| 1:2:1350:G:O2'    | 1:2:1352:G:O6    | 2.20                     | 0.57              |
| 2:C:17:LYS:HD3    | 2:C:173:LEU:HD11 | 1.87                     | 0.57              |
| 7:H:20:PHE:HA     | 7:H:48:TYR:HA    | 1.86                     | 0.57              |
| 37:z:564:G:H2'    | 37:z:565:G:H8    | 1.68                     | 0.57              |
| 1:2:217:U:H2'     | 1:2:218:A:C8     | 2.40                     | 0.57              |
| 1:2:1861:U:P      | 27:b:10:ARG:HH22 | 2.28                     | 0.57              |
| 6:G:100:ARG:NH2   | 6:G:121:TYR:O    | 2.38                     | 0.57              |
| 15:P:22:VAL:HB    | 15:P:23:PRO:HA   | 1.86                     | 0.57              |
| 17:R:137:HIS:NE2  | 36:y:30:G:OP2    | 2.37                     | 0.57              |
| 1:2:1154:G:H2'    | 1:2:1155:G:C8    | 2.39                     | 0.57              |
| 1:2:1240:U:H2'    | 1:2:1241:G:H8    | 1.70                     | 0.57              |
| 3:D:23:ASP:O      | 3:D:27:LYS:NZ    | 2.36                     | 0.57              |
| 3:D:183:GLU:OE1   | 3:D:187:LYS:NZ   | 2.37                     | 0.57              |
| 9:J:6:ALA:HB1     | 9:J:21:SER:HB3   | 1.86                     | 0.57              |
| 9:J:145:ARG:NH2   | 24:Y:50:PHE:O    | 2.38                     | 0.57              |
| 10:K:48:VAL:HG11  | 10:K:54:LYS:HE2  | 1.86                     | 0.57              |
| 19:T:79:GLU:OE2   | 19:T:79:GLU:N    | 2.29                     | 0.57              |
| 20:U:102:GLY:O    | 20:U:106:LYS:N   | 2.33                     | 0.57              |
| 1:2:915:A:H62     | 1:2:1016:A:H2'   | 1.70                     | 0.57              |
| 1:2:1863:A:N6     | 3:D:114:VAL:O    | 2.38                     | 0.57              |
| 2:C:85:ARG:HB2    | 2:C:205:ARG:CZ   | 2.34                     | 0.57              |
| 2:C:122:LEU:HD23  | 2:C:142:LEU:HG   | 1.86                     | 0.57              |
| 8:I:93:LYS:NZ     | 8:I:94:ARG:O     | 2.38                     | 0.57              |
| 10:K:197:PHE:CZ   | 10:K:201:LYS:HD2 | 2.39                     | 0.57              |
| 19:T:123:THR:OG1  | 19:T:124:VAL:N   | 2.38                     | 0.57              |
| 27:b:10:ARG:HB3   | 27:b:33:ASP:O    | 2.05                     | 0.57              |
| 27:b:28:CYS:SG    | 27:b:29:CYS:N    | 2.77                     | 0.57              |
| 29:d:40:ARG:HH21  | 29:d:61:SER:HG   | 1.53                     | 0.57              |
| 2:C:42:LYS:NZ     | 2:C:47:TYR:O     | 2.38                     | 0.57              |
| 2:C:58:LEU:HD21   | 2:C:177:MET:HB3  | 1.86                     | 0.57              |
| 1:2:155:G:H2'     | 1:2:156:G:C8     | 2.39                     | 0.57              |
| 1:2:308:C:H5      | 8:I:183:ARG:HH21 | 1.53                     | 0.57              |
| 1:2:740:G:H1'     | 9:J:109:ARG:HB2  | 1.85                     | 0.57              |
| 5:F:132:LYS:NZ    | 5:F:193:ASP:HB2  | 2.19                     | 0.57              |
| 24:Y:53:ILE:N     | 24:Y:60:LYS:O    | 2.28                     | 0.57              |
| 32:g:173:LEU:HD22 | 32:g:187:ASN:HB3 | 1.85                     | 0.57              |
| 1:2:84:A:N3       | 1:2:150:A:O2'    | 2.36                     | 0.56              |
| 1:2:165:G:H2'     | 1:2:166:A:H8     | 1.70                     | 0.56              |
| 1:2:1595:G:O3'    | 33:h:43:LYS:NZ   | 2.38                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:164:A:H3'     | 1:2:165:G:H21    | 1.69                     | 0.56              |
| 1:2:1798:U:H2'    | 1:2:1799:G:C8    | 2.40                     | 0.56              |
| 3:D:83:LYS:O      | 3:D:104:ASP:N    | 2.34                     | 0.56              |
| 3:D:198:GLU:O     | 3:D:202:GLN:HG3  | 2.04                     | 0.56              |
| 5:F:6:SER:HB3     | 5:F:9:ARG:HD3    | 1.87                     | 0.56              |
| 6:G:11:ARG:N      | 6:G:26:VAL:O     | 2.28                     | 0.56              |
| 6:G:137:PRO:HG2   | 6:G:149:TYR:HA   | 1.85                     | 0.56              |
| 13:N:57:ASP:OD2   | 13:N:60:CYS:N    | 2.38                     | 0.56              |
| 32:g:39:THR:HG22  | 32:g:60:ARG:HG2  | 1.86                     | 0.56              |
| 1:2:630:A:H2'     | 1:2:631:A:C8     | 2.39                     | 0.56              |
| 1:2:1198:U:H2'    | 1:2:1199:G:C8    | 2.41                     | 0.56              |
| 1:2:1271:G:N2     | 1:2:1502:A:OP2   | 2.38                     | 0.56              |
| 1:2:1611:U:OP2    | 17:R:43:ARG:NH1  | 2.34                     | 0.56              |
| 3:D:35:ALA:HB2    | 3:D:44:ILE:HD11  | 1.87                     | 0.56              |
| 8:I:116:LYS:NZ    | 8:I:125:THR:OG1  | 2.36                     | 0.56              |
| 21:V:13:GLU:OE2   | 21:V:16:ARG:NH1  | 2.38                     | 0.56              |
| 26:a:6:THR:HB     | 26:a:28:LEU:HB2  | 1.88                     | 0.56              |
| 27:b:71:LEU:HD13  | 27:b:73:TYR:CE1  | 2.40                     | 0.56              |
| 1:2:642:U:H2'     | 1:2:643:A:H8     | 1.70                     | 0.56              |
| 2:C:144:THR:N     | 2:C:158:ASP:OD2  | 2.34                     | 0.56              |
| 7:H:175:ASP:OD2   | 7:H:179:ASN:ND2  | 2.38                     | 0.56              |
| 14:O:30:GLY:HA2   | 14:O:112:LYS:HD2 | 1.88                     | 0.56              |
| 19:T:15:VAL:O     | 19:T:19:LYS:HG2  | 2.06                     | 0.56              |
| 21:V:76:THR:HG22  | 21:V:94:ARG:HB3  | 1.86                     | 0.56              |
| 22:W:20:ILE:N     | 22:W:91:LEU:O    | 2.29                     | 0.56              |
| 1:2:95:G:H1       | 1:2:425:A:H61    | 1.54                     | 0.56              |
| 1:2:1140:A:H2'    | 1:2:1141:A:C8    | 2.40                     | 0.56              |
| 4:E:133:ALA:O     | 4:E:137:ARG:HG2  | 2.06                     | 0.56              |
| 6:G:182:MET:N     | 6:G:226:PHE:O    | 2.38                     | 0.56              |
| 9:J:99:ARG:HE     | 9:J:100:ILE:H    | 1.54                     | 0.56              |
| 20:U:108:ARG:HH22 | 37:z:530:G:H1'   | 1.70                     | 0.56              |
| 1:2:516:A:H2      | 1:2:549:G:H22    | 1.53                     | 0.56              |
| 1:2:551:A:OP1     | 11:L:171:GLY:N   | 2.29                     | 0.56              |
| 1:2:1854:A:OP1    | 27:b:8:ASN:ND2   | 2.39                     | 0.56              |
| 20:U:114:LEU:O    | 20:U:118:ARG:N   | 2.39                     | 0.56              |
| 24:Y:70:ASN:CG    | 24:Y:71:LYS:HG3  | 2.30                     | 0.56              |
| 32:g:20:GLN:NE2   | 32:g:69:VAL:O    | 2.33                     | 0.56              |
| 1:2:904:A:H2'     | 1:2:905:G:C8     | 2.40                     | 0.56              |
| 1:2:957:G:N2      | 37:z:831:A:N1    | 2.53                     | 0.56              |
| 1:2:1375:A:H2'    | 1:2:1376:C:C6    | 2.41                     | 0.56              |
| 1:2:1409:G:H2'    | 1:2:1410:A:C8    | 2.40                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:10:LYS:HE3    | 9:J:20:GLU:HG2    | 1.87                     | 0.56              |
| 12:M:23:ALA:O     | 12:M:67:PHE:N     | 2.39                     | 0.56              |
| 25:Z:107:ARG:HG3  | 25:Z:110:HIS:HB3  | 1.87                     | 0.56              |
| 1:2:876:G:H2'     | 1:2:877:G:C8      | 2.40                     | 0.56              |
| 20:U:142:ARG:HD2  | 20:U:142:ARG:O    | 2.06                     | 0.56              |
| 22:W:66:ARG:HE    | 22:W:77:TRP:HE1   | 1.54                     | 0.56              |
| 1:2:142:C:N4      | 1:2:319:G:OP2     | 2.39                     | 0.56              |
| 1:2:202:U:H2'     | 1:2:203:G:H8      | 1.69                     | 0.56              |
| 2:C:104:THR:O     | 2:C:107:THR:OG1   | 2.23                     | 0.56              |
| 7:H:194:ASP:OD1   | 7:H:195:GLU:N     | 2.39                     | 0.56              |
| 21:V:28:LEU:HD22  | 21:V:110:LEU:HD11 | 1.87                     | 0.56              |
| 30:e:43:PHE:O     | 30:e:47:ALA:N     | 2.38                     | 0.56              |
| 36:y:27:U:H2'     | 36:y:28:G:C8      | 2.40                     | 0.56              |
| 1:2:389:C:H5''    | 1:2:390:C:C5      | 2.41                     | 0.56              |
| 1:2:1815:U:H2'    | 1:2:1816:A:C8     | 2.41                     | 0.56              |
| 5:F:158:ILE:HD13  | 5:F:205:PRO:HB3   | 1.88                     | 0.56              |
| 6:G:195:ILE:HG23  | 6:G:196:THR:H     | 1.71                     | 0.56              |
| 1:2:1370:C:OP2    | 19:T:7:LYS:NZ     | 2.39                     | 0.55              |
| 1:2:1571:G:H2'    | 1:2:1572:G:C8     | 2.41                     | 0.55              |
| 1:2:1592:C:OP2    | 33:h:85:ARG:NH1   | 2.39                     | 0.55              |
| 1:2:1858:U:O2'    | 1:2:1860:A:N7     | 2.38                     | 0.55              |
| 10:K:3:ILE:HB     | 10:K:30:GLY:HA3   | 1.88                     | 0.55              |
| 12:M:62:PHE:CZ    | 12:M:65:ARG:HA    | 2.41                     | 0.55              |
| 15:P:83:ASP:OD1   | 15:P:84:LEU:N     | 2.37                     | 0.55              |
| 18:S:83:ALA:O     | 18:S:86:GLN:NE2   | 2.39                     | 0.55              |
| 19:T:66:VAL:O     | 19:T:69:ILE:HG22  | 2.06                     | 0.55              |
| 32:g:258:ILE:HG23 | 32:g:267:VAL:HB   | 1.88                     | 0.55              |
| 1:2:77:A:O2'      | 8:I:176:ILE:N     | 2.38                     | 0.55              |
| 1:2:860:A:H2'     | 1:2:861:A:H8      | 1.70                     | 0.55              |
| 1:2:1391:C:H2'    | 1:2:1392:A:N3     | 2.21                     | 0.55              |
| 1:2:1655:C:O5'    | 30:e:32:ARG:NH2   | 2.39                     | 0.55              |
| 22:W:18:HIS:HE1   | 22:W:95:SER:HB2   | 1.71                     | 0.55              |
| 25:Z:72:VAL:HG21  | 25:Z:100:VAL:HG21 | 1.88                     | 0.55              |
| 37:z:570:A:H3'    | 37:z:571:A:H8     | 1.71                     | 0.55              |
| 6:G:49:ARG:NH1    | 6:G:56:LEU:O      | 2.39                     | 0.55              |
| 1:2:21:U:H4'      | 11:L:19:PRO:HG3   | 1.88                     | 0.55              |
| 1:2:1503:G:C8     | 31:f:88:PRO:HD2   | 2.41                     | 0.55              |
| 5:F:46:THR:HB     | 5:F:84:VAL:HA     | 1.87                     | 0.55              |
| 9:J:168:HIS:HE1   | 9:J:169:LYS:HE3   | 1.72                     | 0.55              |
| 13:N:121:GLN:N    | 13:N:124:ASP:OD2  | 2.36                     | 0.55              |
| 32:g:215:GLN:HG2  | 32:g:231:ASP:HA   | 1.89                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:630:A:H2'     | 1:2:631:A:H8     | 1.72                     | 0.55              |
| 1:2:668:U:O4      | 1:2:1023:A:N7    | 2.39                     | 0.55              |
| 1:2:1173:U:H2'    | 1:2:1174:U:C6    | 2.42                     | 0.55              |
| 1:2:1213:A:H2'    | 1:2:1214:C:C6    | 2.42                     | 0.55              |
| 1:2:1294:G:H2'    | 1:2:1295:A:O4'   | 2.07                     | 0.55              |
| 1:2:1427:G:H2'    | 1:2:1428:U:C5    | 2.42                     | 0.55              |
| 11:L:176:LYS:HA   | 11:L:179:LYS:HZ3 | 1.71                     | 0.55              |
| 13:N:101:ARG:HG3  | 25:Z:7:LEU:HA    | 1.89                     | 0.55              |
| 37:z:564:G:H2'    | 37:z:565:G:C8    | 2.41                     | 0.55              |
| 1:2:191:C:H2'     | 1:2:192:U:H6     | 1.72                     | 0.55              |
| 1:2:364:G:H5''    | 13:N:59:LYS:HE3  | 1.89                     | 0.55              |
| 1:2:440:C:OP1     | 6:G:3:ARG:NH2    | 2.39                     | 0.55              |
| 1:2:918:A:OP1     | 24:Y:28:ARG:NH1  | 2.29                     | 0.55              |
| 1:2:1019:A:H2'    | 1:2:1020:A:C8    | 2.41                     | 0.55              |
| 1:2:1687:U:H2'    | 1:2:1688:G:H8    | 1.72                     | 0.55              |
| 10:K:73:THR:O     | 10:K:74:ARG:NH1  | 2.34                     | 0.55              |
| 1:2:526:A:H62     | 1:2:537:G:H21    | 1.53                     | 0.55              |
| 1:2:1045:A:N7     | 1:2:1065:U:O4    | 2.39                     | 0.55              |
| 1:2:1327:C:H4'    | 1:2:1328:A:H5''  | 1.88                     | 0.55              |
| 1:2:1847:C:H2'    | 1:2:1848:U:C6    | 2.42                     | 0.55              |
| 3:D:36:PRO:HB2    | 3:D:38:MET:HE1   | 1.88                     | 0.55              |
| 4:E:187:THR:N     | 4:E:206:ASP:OD2  | 2.40                     | 0.55              |
| 6:G:173:ILE:HG21  | 6:G:227:VAL:HG11 | 1.88                     | 0.55              |
| 13:N:128:VAL:HG12 | 13:N:142:VAL:HA  | 1.88                     | 0.55              |
| 20:U:106:LYS:NZ   | 20:U:109:GLU:OE2 | 2.38                     | 0.55              |
| 27:b:37:LYS:HZ1   | 27:b:70:LYS:HG2  | 1.72                     | 0.55              |
| 1:2:624:A:H2'     | 1:2:625:G:H8     | 1.72                     | 0.55              |
| 1:2:914:U:H3'     | 15:P:64:ARG:HH22 | 1.70                     | 0.55              |
| 1:2:1624:C:H2'    | 1:2:1625:A:H8    | 1.72                     | 0.55              |
| 3:D:144:LYS:HA    | 3:D:208:HIS:ND1  | 2.22                     | 0.55              |
| 7:H:27:ASP:O      | 7:H:29:GLN:NE2   | 2.36                     | 0.55              |
| 20:U:123:LEU:HB3  | 20:U:127:TRP:CZ3 | 2.42                     | 0.55              |
| 37:z:551:C:H2'    | 37:z:552:A:H8    | 1.71                     | 0.55              |
| 37:z:597:A:H2'    | 37:z:598:A:C8    | 2.42                     | 0.55              |
| 1:2:606:A:H5''    | 25:Z:68:LYS:HZ1  | 1.72                     | 0.55              |
| 1:2:1531:G:H2'    | 1:2:1532:A:H8    | 1.72                     | 0.55              |
| 1:2:1704:G:N2     | 1:2:1818:A:N1    | 2.47                     | 0.55              |
| 7:H:40:ALA:HB1    | 7:H:45:TYR:CD2   | 2.42                     | 0.55              |
| 31:f:95:ARG:HG3   | 31:f:97:LYS:H    | 1.70                     | 0.55              |
| 1:2:859:U:O4      | 1:2:860:A:N6     | 2.40                     | 0.55              |
| 1:2:1351:C:H2'    | 1:2:1352:G:C4    | 2.42                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1593:G:OP2    | 33:h:82:SER:OG    | 2.19                     | 0.55              |
| 1:2:1593:G:O6     | 33:h:85:ARG:NH2   | 2.40                     | 0.55              |
| 1:2:1800:A:H2'    | 1:2:1801:C:C6     | 2.42                     | 0.55              |
| 4:E:54:LEU:HG     | 4:E:258:LEU:HD21  | 1.89                     | 0.55              |
| 7:H:77:MET:O      | 7:H:83:ASN:ND2    | 2.39                     | 0.55              |
| 7:H:110:GLN:OE1   | 7:H:110:GLN:N     | 2.37                     | 0.55              |
| 18:S:21:ALA:HA    | 18:S:72:VAL:HG12  | 1.89                     | 0.55              |
| 24:Y:115:GLU:OE2  | 24:Y:118:ARG:NH2  | 2.38                     | 0.55              |
| 30:e:5:GLN:CD     | 30:e:6:LEU:H      | 2.15                     | 0.55              |
| 1:2:146:G:O2'     | 1:2:147:A:H5''    | 2.07                     | 0.54              |
| 1:2:579:G:H5''    | 1:2:580:A:C8      | 2.42                     | 0.54              |
| 1:2:944:C:H2'     | 1:2:945:G:C8      | 2.42                     | 0.54              |
| 1:2:1169:A:H62    | 1:2:1183:G:H21    | 1.56                     | 0.54              |
| 1:2:1289:A:N3     | 31:f:138:ARG:NH1  | 2.55                     | 0.54              |
| 1:2:1445:G:H2'    | 1:2:1446:G:O4'    | 2.06                     | 0.54              |
| 2:C:50:ASN:ND2    | 2:C:53:ARG:HG2    | 2.22                     | 0.54              |
| 9:J:98:ARG:HG3    | 9:J:125:VAL:HG22  | 1.89                     | 0.54              |
| 24:Y:37:PHE:CE1   | 24:Y:41:MET:HE3   | 2.42                     | 0.54              |
| 36:y:50:U:H4'     | 37:z:539:C:H42    | 1.71                     | 0.54              |
| 4:E:108:ARG:NH1   | 4:E:128:CYS:SG    | 2.79                     | 0.54              |
| 7:H:21:GLY:H      | 7:H:48:TYR:HD1    | 1.55                     | 0.54              |
| 10:K:101:ILE:HG22 | 10:K:172:LEU:HD12 | 1.89                     | 0.54              |
| 1:2:619:A:O2'     | 1:2:621:U:OP1     | 2.25                     | 0.54              |
| 1:2:835:C:N4      | 26:a:9:THR:O      | 2.40                     | 0.54              |
| 1:2:1139:A:H5'    | 4:E:175:SER:HB3   | 1.89                     | 0.54              |
| 1:2:1567:C:H2'    | 1:2:1568:G:C8     | 2.42                     | 0.54              |
| 3:D:37:ALA:N      | 3:D:231:LEU:O     | 2.34                     | 0.54              |
| 3:D:208:HIS:CG    | 3:D:208:HIS:O     | 2.61                     | 0.54              |
| 4:E:151:ARG:HB2   | 4:E:233:TYR:HD2   | 1.72                     | 0.54              |
| 6:G:100:ARG:HB2   | 6:G:114:ILE:HD13  | 1.89                     | 0.54              |
| 20:U:143:GLY:O    | 20:U:144:ARG:HD3  | 2.08                     | 0.54              |
| 1:2:743:U:O2'     | 1:2:744:C:O5'     | 2.25                     | 0.54              |
| 1:2:937:C:H2'     | 1:2:938:G:C8      | 2.41                     | 0.54              |
| 1:2:1097:U:H2'    | 1:2:1098:G:C8     | 2.41                     | 0.54              |
| 1:2:1198:U:H2'    | 1:2:1199:G:H8     | 1.71                     | 0.54              |
| 1:2:1640:C:O3'    | 18:S:138:ARG:NE   | 2.41                     | 0.54              |
| 1:2:1728:U:H2'    | 1:2:1729:G:O4'    | 2.07                     | 0.54              |
| 1:2:1775:A:H2'    | 1:2:1776:G:C8     | 2.42                     | 0.54              |
| 3:D:51:ARG:HG3    | 3:D:53:GLN:HE22   | 1.72                     | 0.54              |
| 5:F:135:GLU:N     | 5:F:135:GLU:OE2   | 2.41                     | 0.54              |
| 9:J:41:ARG:HH11   | 9:J:42:GLU:H      | 1.55                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:L:38:ARG:HA    | 34:i:105:ARG:HB3  | 1.88                     | 0.54              |
| 22:W:66:ARG:HE    | 22:W:77:TRP:NE1   | 2.05                     | 0.54              |
| 24:Y:37:PHE:O     | 24:Y:41:MET:HG2   | 2.07                     | 0.54              |
| 26:a:12:PHE:HZ    | 26:a:21:LYS:HD2   | 1.73                     | 0.54              |
| 28:c:1:MET:HG3    | 28:c:5:LYS:HG2    | 1.89                     | 0.54              |
| 31:f:116:ARG:HH12 | 31:f:119:ARG:HA   | 1.72                     | 0.54              |
| 1:2:1000:U:H2'    | 1:2:1001:G:H8     | 1.71                     | 0.54              |
| 1:2:1105:C:H2'    | 1:2:1106:G:O4'    | 2.08                     | 0.54              |
| 1:2:1223:G:C2     | 1:2:1224:A:C8     | 2.96                     | 0.54              |
| 1:2:1244:U:H2'    | 1:2:1245:C:C6     | 2.43                     | 0.54              |
| 1:2:1361:G:H2'    | 1:2:1362:G:H8     | 1.70                     | 0.54              |
| 3:D:133:TYR:CE1   | 3:D:221:PRO:HD2   | 2.42                     | 0.54              |
| 15:P:40:LEU:HD22  | 15:P:50:ILE:HG12  | 1.89                     | 0.54              |
| 32:g:17:TRP:CD1   | 32:g:303:THR:HG1  | 2.25                     | 0.54              |
| 36:y:3:C:H2'      | 36:y:4:A:H8       | 1.72                     | 0.54              |
| 37:z:599:G:H2'    | 37:z:600:G:C8     | 2.42                     | 0.54              |
| 1:2:367:G:OP1     | 10:K:99:ASN:ND2   | 2.41                     | 0.54              |
| 1:2:538:C:H2'     | 1:2:539:C:H6      | 1.73                     | 0.54              |
| 1:2:604:G:H5'     | 34:i:76:VAL:HG22  | 1.89                     | 0.54              |
| 1:2:1552:C:OP1    | 30:e:13:LYS:NZ    | 2.28                     | 0.54              |
| 3:D:162:ARG:HG2   | 3:D:165:ARG:HH21  | 1.72                     | 0.54              |
| 4:E:110:LYS:HD3   | 4:E:128:CYS:HB2   | 1.90                     | 0.54              |
| 9:J:159:ASP:OD1   | 9:J:160:LYS:N     | 2.41                     | 0.54              |
| 16:Q:117:ARG:HD3  | 16:Q:121:ARG:HH21 | 1.73                     | 0.54              |
| 32:g:13:GLY:HA3   | 32:g:43:TRP:CH2   | 2.41                     | 0.54              |
| 33:h:68:ILE:HB    | 33:h:109:TYR:HB2  | 1.88                     | 0.54              |
| 37:z:831:A:H5''   | 37:z:832:A:C4     | 2.43                     | 0.54              |
| 1:2:632:U:H4'     | 1:2:634:G:H4'     | 1.90                     | 0.54              |
| 1:2:1382:A:H2'    | 1:2:1383:G:O4'    | 2.08                     | 0.54              |
| 2:C:125:THR:HG22  | 2:C:147:LEU:HD13  | 1.88                     | 0.54              |
| 6:G:127:ARG:N     | 6:G:140:VAL:O     | 2.33                     | 0.54              |
| 10:K:8:TRP:CD1    | 10:K:22:HIS:HE2   | 2.26                     | 0.54              |
| 11:L:111:GLN:OE1  | 11:L:111:GLN:N    | 2.39                     | 0.54              |
| 18:S:39:LEU:HA    | 18:S:42:ILE:HG12  | 1.90                     | 0.54              |
| 37:z:522:U:H2'    | 37:z:523:G:C8     | 2.43                     | 0.54              |
| 1:2:1260:C:H4'    | 1:2:1261:A:H5'    | 1.89                     | 0.54              |
| 1:2:1560:C:H2'    | 1:2:1561:G:H8     | 1.72                     | 0.54              |
| 1:2:1695:C:N3     | 1:2:1828:A:N6     | 2.56                     | 0.54              |
| 1:2:1700:C:H2'    | 1:2:1701:G:C8     | 2.43                     | 0.54              |
| 7:H:100:ILE:HD11  | 7:H:108:PRO:HB3   | 1.90                     | 0.54              |
| 10:K:6:ASP:OD1    | 10:K:9:HIS:ND1    | 2.41                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:P:52:VAL:HA    | 15:P:55:ARG:HG2   | 1.88                     | 0.54              |
| 18:S:60:LYS:O     | 18:S:64:ALA:N     | 2.41                     | 0.54              |
| 36:y:42:G:H2'     | 36:y:43:A:C8      | 2.42                     | 0.54              |
| 1:2:1099:C:H2'    | 1:2:1100:G:H8     | 1.71                     | 0.54              |
| 3:D:49:VAL:HG12   | 3:D:65:ARG:NH2    | 2.22                     | 0.54              |
| 10:K:190:LEU:HD11 | 10:K:194:GLU:HB3  | 1.90                     | 0.54              |
| 13:N:111:VAL:HG22 | 13:N:140:PHE:HB2  | 1.90                     | 0.54              |
| 17:R:10:ARG:HH12  | 17:R:21:ASP:HA    | 1.72                     | 0.54              |
| 27:b:37:LYS:NZ    | 27:b:71:LEU:O     | 2.35                     | 0.54              |
| 1:2:600:G:H2'     | 1:2:601:G:H8      | 1.73                     | 0.54              |
| 1:2:864:G:N7      | 9:J:115:LYS:HG3   | 2.23                     | 0.54              |
| 22:W:55:ARG:HA    | 22:W:87:ARG:HG3   | 1.88                     | 0.54              |
| 23:X:74:LYS:HA    | 23:X:79:VAL:HG13  | 1.89                     | 0.54              |
| 25:Z:41:PHE:HZ    | 25:Z:102:VAL:HG23 | 1.73                     | 0.54              |
| 32:g:40:ILE:HG13  | 32:g:59:LEU:HB2   | 1.90                     | 0.54              |
| 1:2:191:C:H2'     | 1:2:192:U:C6      | 2.43                     | 0.53              |
| 1:2:977:A:H2'     | 1:2:978:G:C8      | 2.43                     | 0.53              |
| 15:P:30:SER:O     | 15:P:34:LYS:HG2   | 2.07                     | 0.53              |
| 30:e:52:PHE:CZ    | 30:e:54:LYS:HA    | 2.43                     | 0.53              |
| 33:h:66:LYS:HA    | 33:h:111:ARG:HB2  | 1.89                     | 0.53              |
| 35:l:8:LYS:O      | 35:l:12:ARG:HG2   | 2.08                     | 0.53              |
| 2:C:112:ILE:HG13  | 2:C:112:ILE:O     | 2.08                     | 0.53              |
| 7:H:28:VAL:O      | 7:H:42:LYS:NZ     | 2.37                     | 0.53              |
| 8:I:23:LYS:HG2    | 8:I:40:ALA:HB1    | 1.90                     | 0.53              |
| 15:P:19:ARG:HG2   | 15:P:22:VAL:HG13  | 1.89                     | 0.53              |
| 17:R:39:ALA:HA    | 17:R:42:ARG:NE    | 2.23                     | 0.53              |
| 24:Y:7:LEU:HD11   | 24:Y:37:PHE:CD2   | 2.43                     | 0.53              |
| 1:2:403:G:N2      | 1:2:415:G:H1'     | 2.24                     | 0.53              |
| 1:2:1067:G:H2'    | 1:2:1068:U:O4'    | 2.08                     | 0.53              |
| 1:2:1199:G:H2'    | 1:2:1200:A:C8     | 2.43                     | 0.53              |
| 1:2:1648:U:H3     | 1:2:1666:G:H1     | 1.55                     | 0.53              |
| 8:I:76:LEU:HA     | 8:I:94:ARG:HA     | 1.90                     | 0.53              |
| 13:N:135:SER:H    | 13:N:138:VAL:HG12 | 1.73                     | 0.53              |
| 26:a:88:LYS:HB2   | 26:a:97:TYR:HE2   | 1.73                     | 0.53              |
| 37:z:535:A:O2'    | 37:z:540:C:N3     | 2.38                     | 0.53              |
| 1:2:341:G:H2'     | 1:2:342:U:H6      | 1.73                     | 0.53              |
| 1:2:898:G:H2'     | 1:2:899:A:C8      | 2.43                     | 0.53              |
| 1:2:1160:G:H2'    | 1:2:1161:G:N3     | 2.23                     | 0.53              |
| 1:2:1249:A:HO2'   | 1:2:1661:C:HO2'   | 1.50                     | 0.53              |
| 1:2:1403:U:H2'    | 1:2:1404:U:C6     | 2.44                     | 0.53              |
| 12:M:3:MET:HB3    | 12:M:44:HIS:CG    | 2.44                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:1648:U:H2'   | 1:2:1649:G:C8     | 2.43                     | 0.53              |
| 1:2:1736:U:OP1   | 10:K:42:ARG:NH1   | 2.41                     | 0.53              |
| 17:R:78:THR:N    | 17:R:95:GLY:O     | 2.40                     | 0.53              |
| 26:a:114:MET:HE3 | 26:a:114:MET:O    | 2.08                     | 0.53              |
| 1:2:106:C:H2'    | 1:2:107:A:C8      | 2.43                     | 0.53              |
| 9:J:143:ARG:HH12 | 24:Y:53:ILE:HA    | 1.73                     | 0.53              |
| 36:y:46:U:H4'    | 36:y:47:C:C5      | 2.43                     | 0.53              |
| 1:2:642:U:H2'    | 1:2:643:A:C8      | 2.43                     | 0.53              |
| 1:2:1405:A:H2'   | 1:2:1406:C:O4'    | 2.09                     | 0.53              |
| 5:F:62:LYS:HA    | 12:M:96:ARG:HG3   | 1.91                     | 0.53              |
| 22:W:36:CYS:O    | 22:W:40:ILE:N     | 2.40                     | 0.53              |
| 37:z:527:G:N2    | 37:z:563:C:O2'    | 2.39                     | 0.53              |
| 1:2:115:U:O2'    | 1:2:371:C:O2      | 2.19                     | 0.53              |
| 1:2:1015:C:H2'   | 1:2:1016:A:C4     | 2.44                     | 0.53              |
| 1:2:1290:G:H2'   | 1:2:1291:A:C8     | 2.43                     | 0.53              |
| 1:2:1492:U:O2'   | 1:2:1494:A:OP1    | 2.19                     | 0.53              |
| 9:J:143:ARG:HH12 | 24:Y:53:ILE:HG12  | 1.73                     | 0.53              |
| 16:Q:44:VAL:HG13 | 16:Q:53:ILE:HG13  | 1.91                     | 0.53              |
| 33:h:102:LYS:HA  | 33:h:107:VAL:HG12 | 1.91                     | 0.53              |
| 4:E:255:THR:HA   | 4:E:258:LEU:HB2   | 1.89                     | 0.53              |
| 6:G:11:ARG:HA    | 6:G:28:ALA:HB2    | 1.89                     | 0.53              |
| 9:J:145:ARG:N    | 9:J:153:LEU:O     | 2.39                     | 0.53              |
| 9:J:160:LYS:HA   | 9:J:189:PHE:HZ    | 1.74                     | 0.53              |
| 21:V:37:VAL:HG12 | 21:V:39:LEU:H     | 1.73                     | 0.53              |
| 30:e:37:ASN:O    | 30:e:38:MET:HE2   | 2.09                     | 0.53              |
| 1:2:548:G:H2'    | 1:2:549:G:C8      | 2.43                     | 0.53              |
| 1:2:592:G:OP2    | 1:2:593:C:O2'     | 2.25                     | 0.53              |
| 1:2:867:U:OP2    | 15:P:76:LYS:NZ    | 2.32                     | 0.53              |
| 1:2:913:U:H5'    | 9:J:118:ARG:HB2   | 1.90                     | 0.53              |
| 1:2:1029:G:N1    | 1:2:1076:A:O2'    | 2.34                     | 0.53              |
| 1:2:1840:G:O6    | 35:l:8:LYS:NZ     | 2.42                     | 0.53              |
| 3:D:198:GLU:HB2  | 3:D:210:VAL:HG11  | 1.91                     | 0.53              |
| 10:K:162:LEU:HB3 | 10:K:166:PHE:CE2  | 2.44                     | 0.53              |
| 12:M:12:TYR:HB3  | 12:M:83:LEU:HD11  | 1.91                     | 0.53              |
| 15:P:19:ARG:HG3  | 15:P:21:SER:H     | 1.74                     | 0.53              |
| 15:P:70:LYS:O    | 15:P:74:ILE:HD12  | 2.07                     | 0.53              |
| 17:R:18:ARG:H    | 20:U:91:LYS:HA    | 1.73                     | 0.53              |
| 26:a:102:THR:OG1 | 26:a:106:GLN:NE2  | 2.42                     | 0.53              |
| 28:c:1:MET:HG2   | 28:c:3:LEU:H      | 1.73                     | 0.53              |
| 1:2:29:G:H2'     | 1:2:30:C:C6       | 2.45                     | 0.52              |
| 1:2:158:A:H2     | 1:2:453:C:H1'     | 1.72                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:641:U:H2'    | 1:2:642:U:C6      | 2.44                     | 0.52              |
| 8:I:182:PRO:HA   | 8:I:185:LEU:HD12  | 1.90                     | 0.52              |
| 10:K:41:ARG:HE   | 10:K:43:ILE:HD11  | 1.75                     | 0.52              |
| 11:L:87:LEU:HD11 | 11:L:100:LEU:HD11 | 1.91                     | 0.52              |
| 36:y:17:G:O2'    | 36:y:59:A:N1      | 2.36                     | 0.52              |
| 1:2:507:C:H2'    | 1:2:508:G:O4'     | 2.08                     | 0.52              |
| 1:2:577:A:H5'    | 1:2:582:C:C5      | 2.45                     | 0.52              |
| 1:2:819:U:H5     | 11:L:143:ASN:HB2  | 1.74                     | 0.52              |
| 1:2:1044:G:N1    | 1:2:1065:U:OP2    | 2.37                     | 0.52              |
| 2:C:183:LEU:HD12 | 2:C:189:ILE:HD13  | 1.91                     | 0.52              |
| 3:D:227:LYS:O    | 3:D:231:LEU:HG    | 2.09                     | 0.52              |
| 6:G:11:ARG:NE    | 6:G:27:PHE:O      | 2.31                     | 0.52              |
| 16:Q:119:LEU:O   | 16:Q:124:MET:HB2  | 2.09                     | 0.52              |
| 24:Y:11:LEU:O    | 24:Y:15:ASN:ND2   | 2.42                     | 0.52              |
| 27:b:37:LYS:NZ   | 27:b:70:LYS:HG2   | 2.24                     | 0.52              |
| 1:2:1305:C:OP2   | 31:f:105:TYR:OH   | 2.20                     | 0.52              |
| 5:F:132:LYS:HZ3  | 5:F:193:ASP:HB2   | 1.74                     | 0.52              |
| 5:F:138:VAL:O    | 5:F:149:SER:HA    | 2.09                     | 0.52              |
| 7:H:75:SER:O     | 7:H:76:MET:HE2    | 2.10                     | 0.52              |
| 7:H:178:ILE:HG22 | 7:H:182:LYS:HZ2   | 1.75                     | 0.52              |
| 10:K:120:PRO:HB2 | 10:K:123:ARG:HE   | 1.72                     | 0.52              |
| 17:R:32:GLN:HA   | 17:R:35:GLN:HG2   | 1.91                     | 0.52              |
| 37:z:580:U:O4    | 37:z:581:A:N6     | 2.42                     | 0.52              |
| 1:2:549:G:H2'    | 1:2:550:A:H8      | 1.75                     | 0.52              |
| 1:2:942:U:H2'    | 1:2:943:G:C8      | 2.44                     | 0.52              |
| 1:2:1043:C:H2'   | 1:2:1044:G:C8     | 2.44                     | 0.52              |
| 1:2:1283:A:H5'   | 31:f:99:LYS:NZ    | 2.24                     | 0.52              |
| 1:2:1289:A:H2'   | 1:2:1290:G:C8     | 2.44                     | 0.52              |
| 1:2:1428:U:H2'   | 1:2:1429:C:C6     | 2.45                     | 0.52              |
| 1:2:1659:A:H2'   | 1:2:1661:C:H41    | 1.74                     | 0.52              |
| 1:2:1688:G:N2    | 1:2:1828:A:H8     | 2.06                     | 0.52              |
| 2:C:161:ILE:HD12 | 2:C:162:PRO:HD2   | 1.90                     | 0.52              |
| 7:H:106:GLU:OE2  | 7:H:110:GLN:HB2   | 2.09                     | 0.52              |
| 9:J:126:HIS:HA   | 9:J:129:ILE:HG22  | 1.91                     | 0.52              |
| 13:N:96:ILE:HG22 | 13:N:99:TYR:H     | 1.73                     | 0.52              |
| 16:Q:43:HIS:CD2  | 16:Q:55:ARG:HB2   | 2.43                     | 0.52              |
| 32:g:21:ILE:HG22 | 32:g:33:SER:HA    | 1.89                     | 0.52              |
| 32:g:78:ALA:HB3  | 32:g:90:TRP:HB2   | 1.91                     | 0.52              |
| 36:y:10:G:P      | 36:y:45:G:H21     | 2.33                     | 0.52              |
| 1:2:1069:U:H2'   | 1:2:1070:C:C6     | 2.44                     | 0.52              |
| 1:2:1355:U:OP1   | 4:E:99:LYS:NZ     | 2.42                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:1469:G:N2    | 1:2:1471:G:H5''  | 2.24                     | 0.52              |
| 1:2:1668:U:O2'   | 7:H:84:GLY:O     | 2.22                     | 0.52              |
| 3:D:163:GLN:HG3  | 3:D:204:ILE:HD12 | 1.92                     | 0.52              |
| 7:H:121:PRO:HG2  | 7:H:196:LEU:HD12 | 1.91                     | 0.52              |
| 36:y:57:A:O2'    | 36:y:59:A:OP2    | 2.27                     | 0.52              |
| 1:2:1:U:O4       | 11:L:47:LYS:NZ   | 2.33                     | 0.52              |
| 1:2:510:A:H2'    | 1:2:511:A:H8     | 1.74                     | 0.52              |
| 1:2:549:G:H2'    | 1:2:550:A:C8     | 2.44                     | 0.52              |
| 1:2:1444:A:H3'   | 1:2:1445:G:H5''  | 1.92                     | 0.52              |
| 3:D:193:ILE:O    | 3:D:197:ILE:HG13 | 2.10                     | 0.52              |
| 5:F:196:GLY:H    | 5:F:198:ILE:HG13 | 1.74                     | 0.52              |
| 8:I:224:ARG:O    | 8:I:227:GLN:HG3  | 2.10                     | 0.52              |
| 32:g:34:ALA:HB1  | 32:g:66:VAL:HG12 | 1.92                     | 0.52              |
| 35:l:15:ARG:HA   | 35:l:18:ARG:HE   | 1.74                     | 0.52              |
| 1:2:1211:C:H42   | 1:2:1216:A:N6    | 2.07                     | 0.52              |
| 1:2:1652:G:H2'   | 1:2:1653:G:C8    | 2.44                     | 0.52              |
| 9:J:110:THR:HG23 | 9:J:112:ASN:H    | 1.74                     | 0.52              |
| 10:K:191:GLU:HG3 | 13:N:18:GLN:NE2  | 2.25                     | 0.52              |
| 16:Q:142:ARG:HG3 | 27:b:22:ARG:HH21 | 1.73                     | 0.52              |
| 20:U:25:LYS:HA   | 20:U:55:ARG:HA   | 1.92                     | 0.52              |
| 20:U:45:LEU:HD22 | 20:U:50:ILE:HD11 | 1.90                     | 0.52              |
| 1:2:192:U:H3     | 1:2:203:G:H1     | 1.56                     | 0.52              |
| 1:2:868:A:O2'    | 1:2:869:G:H8     | 1.90                     | 0.52              |
| 1:2:1482:A:OP1   | 5:F:151:LYS:HE3  | 2.10                     | 0.52              |
| 1:2:1625:A:H5''  | 20:U:37:GLY:H    | 1.73                     | 0.52              |
| 3:D:165:ARG:O    | 3:D:169:MET:HG2  | 2.10                     | 0.52              |
| 9:J:100:ILE:HG22 | 9:J:125:VAL:HG11 | 1.92                     | 0.52              |
| 10:K:132:GLU:HG2 | 10:K:133:GLU:OE1 | 2.10                     | 0.52              |
| 16:Q:141:ARG:NH1 | 16:Q:142:ARG:O   | 2.43                     | 0.52              |
| 30:e:26:ASN:ND2  | 30:e:27:ARG:O    | 2.43                     | 0.52              |
| 1:2:842:G:OP2    | 6:G:108:ARG:NH2  | 2.43                     | 0.52              |
| 1:2:1043:C:O3'   | 16:Q:141:ARG:NH1 | 2.43                     | 0.52              |
| 1:2:1130:G:H2'   | 1:2:1131:C:C6    | 2.44                     | 0.52              |
| 2:C:85:ARG:NH2   | 19:T:82:ASP:O    | 2.43                     | 0.52              |
| 5:F:5:ILE:HD12   | 5:F:9:ARG:HB3    | 1.91                     | 0.52              |
| 11:L:170:PRO:HB3 | 11:L:174:LYS:HD2 | 1.91                     | 0.52              |
| 12:M:21:MET:HB3  | 12:M:69:TRP:HB2  | 1.92                     | 0.52              |
| 32:g:5:MET:HE3   | 32:g:6:THR:N     | 2.23                     | 0.52              |
| 32:g:132:TRP:HA  | 32:g:139:LYS:H   | 1.73                     | 0.52              |
| 1:2:1388:U:H3    | 1:2:1474:U:H3    | 1.58                     | 0.52              |
| 1:2:1540:A:H2'   | 1:2:1541:G:C8    | 2.45                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:179:ALA:O    | 2:C:183:LEU:HD23  | 2.09                     | 0.52              |
| 3:D:123:ALA:HB3  | 3:D:169:MET:HE3   | 1.92                     | 0.52              |
| 9:J:49:LYS:HG3   | 9:J:63:PHE:HE2    | 1.75                     | 0.52              |
| 20:U:143:GLY:C   | 20:U:144:ARG:HD3  | 2.35                     | 0.52              |
| 22:W:80:PHE:HA   | 30:e:52:PHE:CE2   | 2.45                     | 0.52              |
| 32:g:87:LEU:HD21 | 32:g:111:VAL:HG21 | 1.92                     | 0.52              |
| 1:2:600:G:H2'    | 1:2:601:G:C8      | 2.45                     | 0.51              |
| 1:2:1626:U:O3'   | 20:U:34:LYS:NZ    | 2.39                     | 0.51              |
| 8:I:106:LEU:HD13 | 8:I:109:LEU:HD11  | 1.92                     | 0.51              |
| 12:M:65:ARG:HH12 | 30:e:23:VAL:C     | 2.18                     | 0.51              |
| 18:S:50:LYS:HD3  | 18:S:81:ILE:HD12  | 1.93                     | 0.51              |
| 26:a:91:LEU:HB3  | 26:a:97:TYR:HB3   | 1.92                     | 0.51              |
| 27:b:9:GLY:HA3   | 27:b:12:LYS:HD2   | 1.92                     | 0.51              |
| 1:2:513:A:H62    | 1:2:584:A:H62     | 1.56                     | 0.51              |
| 1:2:544:A:H2'    | 1:2:545:A:C8      | 2.45                     | 0.51              |
| 1:2:858:A:C5     | 24:Y:107:SER:HA   | 2.45                     | 0.51              |
| 1:2:988:A:H2'    | 1:2:989:G:H8      | 1.75                     | 0.51              |
| 1:2:1135:C:H2'   | 1:2:1136:G:O4'    | 2.10                     | 0.51              |
| 1:2:1163:G:H2'   | 1:2:1164:G:O4'    | 2.10                     | 0.51              |
| 3:D:35:ALA:HB3   | 3:D:42:ARG:HA     | 1.92                     | 0.51              |
| 3:D:67:PHE:HB2   | 3:D:86:LEU:HB2    | 1.92                     | 0.51              |
| 8:I:67:VAL:O     | 8:I:100:CYS:N     | 2.42                     | 0.51              |
| 9:J:99:ARG:HH21  | 9:J:100:ILE:HG12  | 1.75                     | 0.51              |
| 11:L:122:SER:H   | 11:L:125:HIS:HB3  | 1.75                     | 0.51              |
| 28:c:35:VAL:HG11 | 28:c:63:LEU:HD11  | 1.92                     | 0.51              |
| 32:g:31:ILE:HG22 | 32:g:45:LEU:HD21  | 1.92                     | 0.51              |
| 32:g:129:ILE:HB  | 32:g:142:VAL:HB   | 1.92                     | 0.51              |
| 1:2:104:A:OP1    | 10:K:12:ARG:NE    | 2.43                     | 0.51              |
| 1:2:947:C:H2'    | 1:2:948:G:C8      | 2.45                     | 0.51              |
| 1:2:1294:G:N3    | 17:R:79:HIS:ND1   | 2.57                     | 0.51              |
| 1:2:1582:G:OP1   | 1:2:1582:G:N2     | 2.43                     | 0.51              |
| 7:H:140:ASP:OD1  | 7:H:141:VAL:N     | 2.42                     | 0.51              |
| 24:Y:30:CYS:SG   | 24:Y:61:ILE:HG12  | 2.50                     | 0.51              |
| 1:2:191:C:H4'    | 1:2:191:C:OP1     | 2.10                     | 0.51              |
| 1:2:664:C:H2'    | 1:2:665:U:C6      | 2.46                     | 0.51              |
| 1:2:1178:A:O3'   | 35:l:15:ARG:NH1   | 2.43                     | 0.51              |
| 1:2:1206:G:H2'   | 1:2:1207:G:H8     | 1.75                     | 0.51              |
| 1:2:1280:A:H4'   | 1:2:1281:G:H5''   | 1.92                     | 0.51              |
| 1:2:1386:U:C2    | 1:2:1477:G:N2     | 2.79                     | 0.51              |
| 1:2:1531:G:H2'   | 1:2:1532:A:C8     | 2.45                     | 0.51              |
| 4:E:181:ILE:HB   | 4:E:208:TYR:HB2   | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:191:SER:HB2   | 4:E:196:LYS:HG3   | 1.91                     | 0.51              |
| 6:G:230:LYS:HB3   | 6:G:233:LYS:HB2   | 1.91                     | 0.51              |
| 6:G:255:ARG:HD3   | 6:G:256:LEU:HD22  | 1.92                     | 0.51              |
| 10:K:114:GLU:HG3  | 10:K:121:LEU:HD23 | 1.92                     | 0.51              |
| 17:R:9:LYS:O      | 20:U:91:LYS:NZ    | 2.38                     | 0.51              |
| 23:X:70:LEU:HD12  | 23:X:71:ARG:HG3   | 1.92                     | 0.51              |
| 28:c:23:ARG:NH1   | 28:c:27:SER:OG    | 2.43                     | 0.51              |
| 34:i:85:LYS:O     | 34:i:89:GLN:NE2   | 2.44                     | 0.51              |
| 1:2:366:A:H2'     | 1:2:367:G:O4'     | 2.10                     | 0.51              |
| 1:2:985:C:H5''    | 3:D:116:LYS:HD2   | 1.93                     | 0.51              |
| 1:2:1093:G:H4'    | 2:C:32:PHE:CG     | 2.45                     | 0.51              |
| 1:2:1281:G:OP1    | 14:O:107:SER:OG   | 2.29                     | 0.51              |
| 1:2:1404:U:OP1    | 18:S:71:ARG:NH1   | 2.44                     | 0.51              |
| 1:2:1660:G:C4     | 21:V:88:MET:HE1   | 2.45                     | 0.51              |
| 2:C:75:SER:O      | 2:C:123:VAL:N     | 2.44                     | 0.51              |
| 9:J:139:ILE:H     | 15:P:19:ARG:HH22  | 1.58                     | 0.51              |
| 16:Q:127:GLY:HA2  | 27:b:58:VAL:HG22  | 1.92                     | 0.51              |
| 20:U:101:ASN:O    | 20:U:105:ASN:ND2  | 2.43                     | 0.51              |
| 32:g:24:THR:HG23  | 32:g:27:PHE:H     | 1.75                     | 0.51              |
| 1:2:151:C:H2'     | 1:2:152:U:H6      | 1.74                     | 0.51              |
| 1:2:562:U:H2'     | 1:2:563:U:C2      | 2.45                     | 0.51              |
| 1:2:967:G:H4'     | 1:2:968:A:H8      | 1.75                     | 0.51              |
| 1:2:1119:C:H4'    | 3:D:149:GLN:HB2   | 1.93                     | 0.51              |
| 2:C:178:LEU:O     | 2:C:182:VAL:HG22  | 2.11                     | 0.51              |
| 6:G:69:PHE:CG     | 26:a:17:LEU:HD11  | 2.46                     | 0.51              |
| 12:M:36:ALA:HB1   | 12:M:39:ASN:HD21  | 1.74                     | 0.51              |
| 17:R:30:TYR:HA    | 17:R:33:LEU:HB3   | 1.92                     | 0.51              |
| 32:g:206:LEU:HD21 | 32:g:218:LEU:HD12 | 1.91                     | 0.51              |
| 1:2:16:G:H2'      | 1:2:17:C:C6       | 2.46                     | 0.51              |
| 1:2:449:C:H3'     | 1:2:450:A:H8      | 1.76                     | 0.51              |
| 1:2:1097:U:H2'    | 1:2:1098:G:H8     | 1.76                     | 0.51              |
| 1:2:1511:G:O3'    | 17:R:122:THR:OG1  | 2.24                     | 0.51              |
| 4:E:195:PRO:HA    | 4:E:198:LEU:HG    | 1.92                     | 0.51              |
| 5:F:167:TYR:OH    | 5:F:201:LYS:O     | 2.26                     | 0.51              |
| 11:L:52:LYS:HA    | 11:L:55:LYS:HE3   | 1.93                     | 0.51              |
| 23:X:62:MET:HE3   | 23:X:62:MET:O     | 2.11                     | 0.51              |
| 23:X:64:GLU:HG2   | 28:c:3:LEU:HD23   | 1.93                     | 0.51              |
| 26:a:24:VAL:HB    | 26:a:72:PHE:HD1   | 1.75                     | 0.51              |
| 32:g:64:HIS:ND1   | 32:g:83:TRP:HB2   | 2.26                     | 0.51              |
| 37:z:521:U:H2'    | 37:z:522:U:C6     | 2.45                     | 0.51              |
| 37:z:541:C:H2'    | 37:z:542:A:C8     | 2.45                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:369:C:H2'    | 1:2:370:G:C8      | 2.46                     | 0.51              |
| 1:2:628:C:H2'    | 1:2:629:C:C6      | 2.44                     | 0.51              |
| 1:2:736:C:O4'    | 9:J:99:ARG:NH2    | 2.44                     | 0.51              |
| 1:2:1634:G:H21   | 36:y:41:A:H4'     | 1.76                     | 0.51              |
| 1:2:1796:C:H2'   | 1:2:1797:U:H6     | 1.76                     | 0.51              |
| 3:D:151:ARG:HD3  | 3:D:152:LYS:H     | 1.75                     | 0.51              |
| 6:G:184:THR:HG22 | 6:G:224:ASN:HA    | 1.92                     | 0.51              |
| 10:K:191:GLU:HG3 | 13:N:18:GLN:HE21  | 1.75                     | 0.51              |
| 20:U:80:PRO:HB2  | 20:U:82:TRP:NE1   | 2.26                     | 0.51              |
| 23:X:38:GLU:N    | 23:X:38:GLU:OE1   | 2.44                     | 0.51              |
| 24:Y:78:ARG:NH1  | 24:Y:126:LEU:HD13 | 2.26                     | 0.51              |
| 32:g:5:MET:HE2   | 32:g:310:TRP:HB3  | 1.93                     | 0.51              |
| 32:g:41:ILE:HD13 | 32:g:55:PRO:HB3   | 1.92                     | 0.51              |
| 1:2:1013:U:H2'   | 1:2:1014:U:H6     | 1.75                     | 0.51              |
| 1:2:1537:C:O2'   | 18:S:43:GLU:OE1   | 2.24                     | 0.51              |
| 1:2:1796:C:H2'   | 1:2:1797:U:C6     | 2.45                     | 0.51              |
| 2:C:181:GLU:O    | 2:C:185:MET:HG2   | 2.11                     | 0.51              |
| 7:H:50:PRO:HB3   | 7:H:69:VAL:HG12   | 1.93                     | 0.51              |
| 9:J:144:ILE:HA   | 9:J:154:ILE:HA    | 1.92                     | 0.51              |
| 14:O:52:LEU:N    | 14:O:77:ILE:O     | 2.39                     | 0.51              |
| 22:W:70:CYS:H    | 30:e:40:ARG:NH2   | 2.09                     | 0.51              |
| 26:a:21:LYS:HB2  | 26:a:75:ILE:HB    | 1.92                     | 0.51              |
| 1:2:624:A:H2'    | 1:2:625:G:C8      | 2.45                     | 0.51              |
| 2:C:80:ARG:O     | 2:C:84:GLN:NE2    | 2.41                     | 0.51              |
| 3:D:49:VAL:HG11  | 3:D:62:LEU:HB2    | 1.92                     | 0.51              |
| 4:E:218:LEU:HA   | 4:E:221:PHE:CB    | 2.41                     | 0.51              |
| 15:P:49:GLN:HA   | 15:P:52:VAL:HG22  | 1.94                     | 0.51              |
| 32:g:216:ALA:HB3 | 32:g:230:LEU:HB2  | 1.92                     | 0.51              |
| 1:2:663:G:H2'    | 1:2:664:C:C6      | 2.46                     | 0.50              |
| 1:2:1236:A:C4    | 17:R:100:LYS:HE2  | 2.47                     | 0.50              |
| 1:2:1718:G:H2'   | 1:2:1719:A:H8     | 1.76                     | 0.50              |
| 20:U:120:HIS:O   | 20:U:124:ARG:HG2  | 2.10                     | 0.50              |
| 1:2:4:C:H1'      | 11:L:18:ARG:NH2   | 2.23                     | 0.50              |
| 1:2:96:C:H2'     | 1:2:97:U:H6       | 1.75                     | 0.50              |
| 1:2:987:G:C6     | 1:2:1130:G:H4'    | 2.45                     | 0.50              |
| 1:2:1164:G:H2'   | 1:2:1165:G:O4'    | 2.11                     | 0.50              |
| 28:c:61:THR:HG23 | 28:c:62:VAL:HG23  | 1.92                     | 0.50              |
| 32:g:155:ARG:HG2 | 32:g:198:VAL:HG23 | 1.94                     | 0.50              |
| 32:g:290:ALA:HB3 | 32:g:299:PHE:HB2  | 1.94                     | 0.50              |
| 1:2:28:U:H2'     | 1:2:29:G:C8       | 2.46                     | 0.50              |
| 1:2:411:G:H5'    | 13:N:98:LYS:HG3   | 1.93                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:454:A:H3'     | 1:2:455:A:H8     | 1.76                     | 0.50              |
| 1:2:794:G:N7      | 9:J:106:ARG:HA   | 2.27                     | 0.50              |
| 1:2:1069:U:H2'    | 1:2:1070:C:H6    | 1.76                     | 0.50              |
| 1:2:1266:G:O6     | 1:2:1507:U:O4    | 2.29                     | 0.50              |
| 1:2:1268:C:OP1    | 31:f:94:LYS:NZ   | 2.45                     | 0.50              |
| 1:2:1615:A:H2'    | 17:R:40:ARG:NH2  | 2.26                     | 0.50              |
| 1:2:1623:C:H2'    | 1:2:1624:C:C6    | 2.46                     | 0.50              |
| 1:2:1643:G:H5'    | 18:S:126:ARG:O   | 2.12                     | 0.50              |
| 16:Q:37:PHE:HE1   | 16:Q:110:PRO:HD3 | 1.75                     | 0.50              |
| 23:X:3:SER:OG     | 23:X:7:GLU:HG3   | 2.11                     | 0.50              |
| 27:b:10:ARG:H     | 27:b:12:LYS:NZ   | 2.09                     | 0.50              |
| 31:f:105:TYR:HB2  | 31:f:131:PHE:HE2 | 1.76                     | 0.50              |
| 33:h:57:LYS:HG2   | 33:h:77:LEU:HD21 | 1.92                     | 0.50              |
| 1:2:365:U:O2'     | 13:N:7:GLU:OE2   | 2.18                     | 0.50              |
| 1:2:389:C:H5''    | 1:2:390:C:H5     | 1.75                     | 0.50              |
| 1:2:856:G:H21     | 24:Y:107:SER:HB3 | 1.76                     | 0.50              |
| 1:2:1220:G:H1     | 1:2:1637:U:H3    | 1.60                     | 0.50              |
| 1:2:1537:C:H2'    | 1:2:1538:U:C2    | 2.47                     | 0.50              |
| 1:2:1612:G:O6     | 17:R:43:ARG:NE   | 2.38                     | 0.50              |
| 10:K:88:ASN:OD1   | 10:K:205:ARG:NH1 | 2.43                     | 0.50              |
| 20:U:98:VAL:HG11  | 20:U:106:LYS:HG2 | 1.92                     | 0.50              |
| 24:Y:35:VAL:O     | 24:Y:39:THR:HG23 | 2.11                     | 0.50              |
| 28:c:37:CYS:SG    | 28:c:60:SER:OG   | 2.64                     | 0.50              |
| 1:2:116:U:O4      | 1:2:337:G:O6     | 2.30                     | 0.50              |
| 1:2:495:G:H2'     | 1:2:496:G:H8     | 1.77                     | 0.50              |
| 1:2:792:G:H2'     | 1:2:793:C:C6     | 2.46                     | 0.50              |
| 1:2:1799:G:H2'    | 1:2:1800:A:C8    | 2.47                     | 0.50              |
| 5:F:50:ILE:HG22   | 5:F:88:ALA:HA    | 1.93                     | 0.50              |
| 6:G:133:THR:O     | 6:G:136:ILE:HG13 | 2.12                     | 0.50              |
| 6:G:238:LEU:O     | 6:G:242:LYS:NZ   | 2.44                     | 0.50              |
| 24:Y:10:ALA:O     | 24:Y:14:ILE:HD12 | 2.11                     | 0.50              |
| 31:f:132:MET:HG2  | 31:f:141:CYS:HB2 | 1.93                     | 0.50              |
| 32:g:154:VAL:O    | 32:g:155:ARG:NH1 | 2.40                     | 0.50              |
| 1:2:370:G:H5''    | 10:K:31:ARG:HH21 | 1.77                     | 0.50              |
| 1:2:1854:A:H5''   | 27:b:8:ASN:HD21  | 1.77                     | 0.50              |
| 2:C:85:ARG:HG2    | 2:C:89:LYS:NZ    | 2.26                     | 0.50              |
| 9:J:67:PRO:HG2    | 9:J:68:GLN:OE1   | 2.11                     | 0.50              |
| 10:K:100:CYS:SG   | 10:K:101:ILE:N   | 2.85                     | 0.50              |
| 18:S:146:ARG:HH21 | 36:y:31:C:P      | 2.35                     | 0.50              |
| 20:U:80:PRO:HB2   | 20:U:82:TRP:CD1  | 2.47                     | 0.50              |
| 24:Y:41:MET:HE1   | 24:Y:129:PHE:CD1 | 2.46                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:a:40:ILE:HA    | 26:a:43:LYS:HZ3   | 1.76                     | 0.50              |
| 1:2:1685:U:H2'    | 1:2:1686:U:H6     | 1.77                     | 0.50              |
| 1:2:1710:A:N1     | 1:2:1812:A:H2     | 2.10                     | 0.50              |
| 1:2:1792:C:O2'    | 10:K:2:GLY:N      | 2.45                     | 0.50              |
| 2:C:77:ILE:HG22   | 2:C:123:VAL:O     | 2.12                     | 0.50              |
| 13:N:84:ARG:N     | 13:N:84:ARG:HD2   | 2.27                     | 0.50              |
| 19:T:99:ASP:OD1   | 19:T:102:THR:OG1  | 2.29                     | 0.50              |
| 25:Z:59:ALA:N     | 25:Z:65:ALA:O     | 2.42                     | 0.50              |
| 30:e:27:ARG:HA    | 30:e:30:LEU:HD23  | 1.94                     | 0.50              |
| 32:g:206:LEU:HD11 | 32:g:218:LEU:HB3  | 1.93                     | 0.50              |
| 1:2:444:U:O3'     | 8:I:94:ARG:NH2    | 2.32                     | 0.50              |
| 1:2:552:U:H2'     | 1:2:553:G:C8      | 2.47                     | 0.50              |
| 1:2:742:C:H2'     | 1:2:743:U:C6      | 2.47                     | 0.50              |
| 1:2:1743:G:O6     | 1:2:1780:U:O4     | 2.30                     | 0.50              |
| 8:I:27:PHE:HA     | 8:I:30:LYS:HD2    | 1.92                     | 0.50              |
| 8:I:37:ALA:HA     | 8:I:49:VAL:HA     | 1.94                     | 0.50              |
| 17:R:11:THR:HA    | 17:R:16:THR:HG22  | 1.93                     | 0.50              |
| 24:Y:101:PHE:HB2  | 24:Y:129:PHE:CZ   | 2.46                     | 0.50              |
| 24:Y:104:LEU:HB3  | 24:Y:125:ILE:HD12 | 1.92                     | 0.50              |
| 1:2:98:C:OP2      | 1:2:416:A:O2'     | 2.30                     | 0.50              |
| 1:2:374:U:H4'     | 13:N:134:LEU:O    | 2.12                     | 0.50              |
| 1:2:381:C:H2'     | 1:2:382:A:H8      | 1.77                     | 0.50              |
| 1:2:545:A:H2'     | 1:2:546:U:C6      | 2.47                     | 0.50              |
| 1:2:797:U:H2'     | 1:2:798:A:H8      | 1.76                     | 0.50              |
| 1:2:1491:G:N2     | 30:e:45:GLN:OE1   | 2.41                     | 0.50              |
| 2:C:198:MET:HE2   | 19:T:89:SER:HB3   | 1.94                     | 0.50              |
| 3:D:137:LEU:HD11  | 3:D:176:VAL:HG21  | 1.93                     | 0.50              |
| 14:O:40:LYS:HZ1   | 14:O:44:LYS:HE3   | 1.76                     | 0.50              |
| 29:d:31:ARG:HH11  | 29:d:43:ILE:HG12  | 1.77                     | 0.50              |
| 1:2:944:C:H2'     | 1:2:945:G:H8      | 1.76                     | 0.49              |
| 1:2:1718:G:H2'    | 1:2:1719:A:C8     | 2.47                     | 0.49              |
| 2:C:89:LYS:CE     | 2:C:201:LEU:HG    | 2.40                     | 0.49              |
| 5:F:203:PRO:HA    | 5:F:208:VAL:HG13  | 1.94                     | 0.49              |
| 6:G:54:TYR:HH     | 26:a:17:LEU:H     | 1.59                     | 0.49              |
| 13:N:35:ARG:NH2   | 13:N:53:GLY:O     | 2.45                     | 0.49              |
| 32:g:251:ALA:HB2  | 32:g:289:LEU:HD23 | 1.94                     | 0.49              |
| 37:z:560:C:H2'    | 37:z:561:U:H6     | 1.76                     | 0.49              |
| 1:2:291:U:H2'     | 1:2:292:A:C8      | 2.47                     | 0.49              |
| 1:2:332:C:C2      | 1:2:333:A:C8      | 3.00                     | 0.49              |
| 1:2:853:U:H4'     | 6:G:201:HIS:NE2   | 2.27                     | 0.49              |
| 1:2:1193:G:H2'    | 1:2:1194:G:H8     | 1.77                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:111:CYS:HA   | 3:D:114:VAL:HG12  | 1.94                     | 0.49              |
| 5:F:127:MET:HE1  | 5:F:133:GLY:HA2   | 1.93                     | 0.49              |
| 5:F:225:GLU:O    | 5:F:227:LYS:NZ    | 2.42                     | 0.49              |
| 16:Q:91:THR:HA   | 16:Q:124:MET:HE1  | 1.94                     | 0.49              |
| 24:Y:105:THR:HB  | 24:Y:126:LEU:HD21 | 1.94                     | 0.49              |
| 26:a:45:ALA:O    | 26:a:49:LYS:N     | 2.45                     | 0.49              |
| 32:g:125:ARG:HG2 | 32:g:150:TRP:CD2  | 2.47                     | 0.49              |
| 32:g:251:ALA:HA  | 32:g:256:ILE:HD12 | 1.94                     | 0.49              |
| 1:2:149:A:C5     | 1:2:170:A:N6      | 2.80                     | 0.49              |
| 1:2:349:U:C5'    | 25:Z:22:TRP:HH2   | 2.26                     | 0.49              |
| 1:2:1123:C:H2'   | 1:2:1124:C:C6     | 2.47                     | 0.49              |
| 1:2:1711:C:H2'   | 1:2:1712:C:H6     | 1.76                     | 0.49              |
| 6:G:136:ILE:HG23 | 6:G:149:TYR:CE1   | 2.47                     | 0.49              |
| 11:L:106:LEU:HA  | 11:L:109:ARG:HG3  | 1.93                     | 0.49              |
| 23:X:21:ASN:HD21 | 24:Y:66:THR:HB    | 1.77                     | 0.49              |
| 24:Y:41:MET:HE1  | 24:Y:129:PHE:CE1  | 2.48                     | 0.49              |
| 24:Y:101:PHE:HA  | 24:Y:113:HIS:NE2  | 2.27                     | 0.49              |
| 25:Z:1:MET:SD    | 25:Z:3:LYS:NZ     | 2.72                     | 0.49              |
| 1:2:445:A:H2'    | 1:2:446:C:C6      | 2.47                     | 0.49              |
| 1:2:865:A:C5     | 1:2:911:G:H1'     | 2.47                     | 0.49              |
| 1:2:1395:C:H5''  | 32:g:100:ARG:CZ   | 2.42                     | 0.49              |
| 1:2:1537:C:OP1   | 21:V:63:HIS:NE2   | 2.45                     | 0.49              |
| 1:2:1668:U:OP2   | 18:S:17:LYS:HD2   | 2.13                     | 0.49              |
| 5:F:46:THR:N     | 5:F:83:SER:O      | 2.44                     | 0.49              |
| 13:N:93:LEU:HD23 | 13:N:93:LEU:H     | 1.77                     | 0.49              |
| 16:Q:27:VAL:HG23 | 16:Q:91:THR:H     | 1.77                     | 0.49              |
| 18:S:124:PRO:O   | 18:S:126:ARG:NH1  | 2.45                     | 0.49              |
| 37:z:574:C:O2'   | 37:z:575:A:OP1    | 2.25                     | 0.49              |
| 1:2:158:A:C2     | 1:2:453:C:H1'     | 2.48                     | 0.49              |
| 1:2:232:A:H2'    | 1:2:233:A:C8      | 2.47                     | 0.49              |
| 1:2:551:A:H2'    | 1:2:552:U:C6      | 2.47                     | 0.49              |
| 1:2:1278:A:H62   | 14:O:101:ARG:HB3  | 1.76                     | 0.49              |
| 1:2:1583:A:H2'   | 1:2:1584:A:O4'    | 2.12                     | 0.49              |
| 1:2:1803:A:H2'   | 1:2:1804:U:C6     | 2.48                     | 0.49              |
| 1:2:1836:C:H2'   | 1:2:1837:G:H8     | 1.78                     | 0.49              |
| 2:C:199:PRO:HG2  | 19:T:91:LEU:HD11  | 1.93                     | 0.49              |
| 4:E:235:TYR:OH   | 24:Y:71:LYS:HD2   | 2.12                     | 0.49              |
| 4:E:236:LEU:HD21 | 24:Y:70:ASN:CG    | 2.38                     | 0.49              |
| 7:H:188:TYR:HA   | 7:H:191:LYS:HE2   | 1.95                     | 0.49              |
| 10:K:39:GLY:O    | 10:K:61:ASP:HB2   | 2.13                     | 0.49              |
| 18:S:86:GLN:O    | 18:S:90:LYS:HG2   | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:a:38:THR:HA    | 26:a:41:GLN:HG2   | 1.93                     | 0.49              |
| 32:g:155:ARG:HG3  | 32:g:199:THR:HA   | 1.94                     | 0.49              |
| 1:2:96:C:H2'      | 1:2:97:U:C6       | 2.47                     | 0.49              |
| 1:2:190:A:H3'     | 1:2:191:C:H5''    | 1.94                     | 0.49              |
| 1:2:904:A:H2'     | 1:2:905:G:H8      | 1.77                     | 0.49              |
| 1:2:1128:C:H2'    | 1:2:1129:A:O4'    | 2.13                     | 0.49              |
| 1:2:1451:A:H2'    | 1:2:1452:G:H8     | 1.77                     | 0.49              |
| 1:2:1453:U:H2'    | 1:2:1454:G:C8     | 2.48                     | 0.49              |
| 1:2:1553:C:H2'    | 1:2:1554:C:C6     | 2.48                     | 0.49              |
| 13:N:77:VAL:HG22  | 13:N:86:ILE:HD11  | 1.93                     | 0.49              |
| 16:Q:142:ARG:NH2  | 27:b:28:CYS:O     | 2.45                     | 0.49              |
| 17:R:10:ARG:NH2   | 17:R:20:VAL:O     | 2.43                     | 0.49              |
| 19:T:27:ASP:OD2   | 19:T:30:THR:N     | 2.38                     | 0.49              |
| 19:T:109:LEU:HG   | 19:T:111:PHE:CD2  | 2.46                     | 0.49              |
| 27:b:73:TYR:HE2   | 27:b:83:VAL:HG11  | 1.78                     | 0.49              |
| 28:c:11:SER:HB2   | 28:c:15:GLU:HB2   | 1.93                     | 0.49              |
| 32:g:206:LEU:HD11 | 32:g:218:LEU:HD12 | 1.93                     | 0.49              |
| 36:y:12:G:C6      | 36:y:23:G:C6      | 3.01                     | 0.49              |
| 37:z:831:A:H5''   | 37:z:832:A:C5     | 2.47                     | 0.49              |
| 1:2:193:C:H2'     | 1:2:194:C:C6      | 2.47                     | 0.49              |
| 1:2:495:G:H2'     | 1:2:496:G:C8      | 2.48                     | 0.49              |
| 1:2:599:U:H2'     | 1:2:600:G:H8      | 1.77                     | 0.49              |
| 1:2:1313:U:H2'    | 1:2:1314:G:C8     | 2.47                     | 0.49              |
| 1:2:1769:U:H2'    | 1:2:1770:G:C8     | 2.48                     | 0.49              |
| 2:C:50:ASN:HD22   | 2:C:53:ARG:HG2    | 1.77                     | 0.49              |
| 32:g:33:SER:HB3   | 32:g:43:TRP:HE1   | 1.77                     | 0.49              |
| 32:g:87:LEU:HD11  | 32:g:108:VAL:HG21 | 1.95                     | 0.49              |
| 1:2:121:U:O3'     | 6:G:77:ARG:NH2    | 2.46                     | 0.49              |
| 1:2:148:U:O4      | 1:2:170:A:N7      | 2.46                     | 0.49              |
| 1:2:869:G:H5''    | 13:N:156:GLN:HG2  | 1.95                     | 0.49              |
| 1:2:1320:G:H2'    | 1:2:1321:G:C8     | 2.48                     | 0.49              |
| 1:2:1596:A:O5'    | 33:h:41:ARG:NH2   | 2.45                     | 0.49              |
| 4:E:194:VAL:HG23  | 4:E:195:PRO:HD3   | 1.94                     | 0.49              |
| 8:I:4:ASN:HB3     | 8:I:110:ASN:HD22  | 1.78                     | 0.49              |
| 18:S:55:VAL:HA    | 18:S:63:PHE:CE2   | 2.48                     | 0.49              |
| 18:S:146:ARG:HE   | 36:y:31:C:P       | 2.35                     | 0.49              |
| 32:g:207:CYS:N    | 32:g:219:TRP:O    | 2.33                     | 0.49              |
| 1:2:107:A:H2'     | 1:2:108:G:C8      | 2.48                     | 0.49              |
| 1:2:1450:A:N7     | 1:2:1472:A:N6     | 2.61                     | 0.49              |
| 1:2:1674:A:N6     | 7:H:58:ALA:H      | 2.11                     | 0.49              |
| 3:D:218:LEU:O     | 3:D:219:LYS:HE2   | 2.13                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:J:65:PRO:HB2   | 9:J:67:PRO:HD3    | 1.95                     | 0.49              |
| 13:N:119:ASP:N   | 13:N:119:ASP:OD1  | 2.46                     | 0.49              |
| 31:f:135:HIS:HD2 | 31:f:140:TYR:H    | 1.61                     | 0.49              |
| 1:2:67:C:N4      | 1:2:151:C:HO2'    | 2.10                     | 0.49              |
| 1:2:162:C:H2'    | 1:2:163:U:O4'     | 2.12                     | 0.49              |
| 1:2:189:G:O2'    | 1:2:205:G:N2      | 2.38                     | 0.49              |
| 1:2:389:C:N3     | 13:N:104:LYS:NZ   | 2.57                     | 0.49              |
| 1:2:413:U:H2'    | 1:2:414:C:C6      | 2.48                     | 0.49              |
| 1:2:547:U:C2     | 1:2:548:G:C8      | 3.00                     | 0.49              |
| 1:2:831:C:H3'    | 26:a:8:ARG:HH22   | 1.78                     | 0.49              |
| 1:2:930:G:H22    | 1:2:1004:A:H2     | 1.60                     | 0.49              |
| 1:2:1151:U:O2'   | 1:2:1152:U:H5'    | 2.13                     | 0.49              |
| 1:2:1707:A:H2'   | 1:2:1708:C:C6     | 2.48                     | 0.49              |
| 7:H:20:PHE:HB3   | 7:H:23:TRP:HB2    | 1.95                     | 0.49              |
| 7:H:160:GLU:HA   | 7:H:163:PHE:HB2   | 1.94                     | 0.49              |
| 9:J:68:GLN:HB3   | 9:J:71:SER:HB2    | 1.95                     | 0.49              |
| 11:L:61:LEU:HD11 | 11:L:95:ASP:HA    | 1.94                     | 0.49              |
| 12:M:27:VAL:HG12 | 12:M:43:LEU:HD21  | 1.93                     | 0.49              |
| 17:R:83:MET:HA   | 17:R:83:MET:HE3   | 1.94                     | 0.49              |
| 18:S:86:GLN:O    | 18:S:89:SER:OG    | 2.28                     | 0.49              |
| 1:2:993:A:H2'    | 1:2:994:A:C8      | 2.48                     | 0.48              |
| 1:2:1000:U:H2'   | 1:2:1001:G:C8     | 2.47                     | 0.48              |
| 1:2:1045:A:O2'   | 1:2:1848:U:O2     | 2.27                     | 0.48              |
| 1:2:1397:A:H4'   | 22:W:52:GLY:HA3   | 1.94                     | 0.48              |
| 1:2:1429:C:H2'   | 1:2:1430:C:C6     | 2.48                     | 0.48              |
| 10:K:151:GLU:HB2 | 10:K:152:ARG:HH11 | 1.77                     | 0.48              |
| 11:L:54:ARG:NH1  | 11:L:98:LEU:HG    | 2.28                     | 0.48              |
| 12:M:1:MET:H1    | 12:M:3:MET:N      | 2.11                     | 0.48              |
| 25:Z:60:LYS:HE3  | 25:Z:116:PRO:HB3  | 1.95                     | 0.48              |
| 27:b:10:ARG:H    | 27:b:12:LYS:HZ3   | 1.60                     | 0.48              |
| 37:z:520:U:H2'   | 37:z:521:U:C6     | 2.48                     | 0.48              |
| 1:2:164:A:H3'    | 1:2:165:G:N2      | 2.28                     | 0.48              |
| 1:2:217:U:H2'    | 1:2:218:A:H8      | 1.76                     | 0.48              |
| 1:2:521:A:H2'    | 1:2:522:C:C6      | 2.48                     | 0.48              |
| 1:2:606:A:H5''   | 25:Z:68:LYS:NZ    | 2.28                     | 0.48              |
| 1:2:1663:U:OP2   | 18:S:141:TYR:OH   | 2.31                     | 0.48              |
| 6:G:251:GLU:O    | 6:G:254:LYS:HG2   | 2.13                     | 0.48              |
| 7:H:55:ARG:NH2   | 18:S:123:ASP:OD1  | 2.47                     | 0.48              |
| 9:J:104:PRO:HD3  | 9:J:116:ARG:NH1   | 2.28                     | 0.48              |
| 11:L:132:GLN:HG3 | 11:L:134:HIS:CD2  | 2.48                     | 0.48              |
| 12:M:57:TYR:HA   | 12:M:74:GLU:HG3   | 1.95                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:W:66:ARG:HA   | 22:W:77:TRP:CD1   | 2.48                     | 0.48              |
| 32:g:131:LEU:O   | 32:g:139:LYS:N    | 2.46                     | 0.48              |
| 1:2:64:A:N6      | 1:2:83:A:OP2      | 2.34                     | 0.48              |
| 1:2:151:C:N3     | 1:2:168:C:N4      | 2.58                     | 0.48              |
| 1:2:874:G:C6     | 1:2:904:A:N1      | 2.81                     | 0.48              |
| 1:2:959:A:H2'    | 1:2:960:A:C8      | 2.48                     | 0.48              |
| 1:2:1424:G:C2    | 1:2:1425:G:C8     | 3.01                     | 0.48              |
| 1:2:1668:U:H2'   | 1:2:1669:G:O4'    | 2.14                     | 0.48              |
| 5:F:201:LYS:HZ3  | 5:F:203:PRO:HB2   | 1.77                     | 0.48              |
| 13:N:11:GLN:HB2  | 13:N:56:ILE:HG13  | 1.95                     | 0.48              |
| 19:T:29:HIS:HA   | 19:T:32:LYS:HE3   | 1.94                     | 0.48              |
| 20:U:23:ARG:NH1  | 33:h:48:VAL:HG22  | 2.28                     | 0.48              |
| 31:f:135:HIS:HB2 | 31:f:138:ARG:HB2  | 1.94                     | 0.48              |
| 35:l:20:MET:HA   | 35:l:23:ARG:HE    | 1.79                     | 0.48              |
| 37:z:535:A:O2'   | 37:z:541:C:N4     | 2.47                     | 0.48              |
| 1:2:531:U:H2'    | 1:2:532:U:C6      | 2.48                     | 0.48              |
| 1:2:625:G:H2'    | 1:2:626:C:C6      | 2.47                     | 0.48              |
| 1:2:927:C:H2'    | 1:2:928:G:C8      | 2.49                     | 0.48              |
| 1:2:1562:G:H2'   | 1:2:1563:C:C6     | 2.47                     | 0.48              |
| 1:2:1563:C:H2'   | 1:2:1564:A:C4     | 2.48                     | 0.48              |
| 6:G:246:LEU:HD21 | 6:G:250:GLU:HG3   | 1.95                     | 0.48              |
| 17:R:10:ARG:NH1  | 17:R:21:ASP:HA    | 2.29                     | 0.48              |
| 19:T:83:ASN:OD1  | 19:T:84:TYR:N     | 2.46                     | 0.48              |
| 24:Y:86:LEU:HD23 | 24:Y:117:ARG:HH21 | 1.78                     | 0.48              |
| 31:f:106:TYR:CD1 | 31:f:114:ILE:HD12 | 2.48                     | 0.48              |
| 37:z:541:C:H2'   | 37:z:542:A:H8     | 1.78                     | 0.48              |
| 1:2:19:A:H5'     | 25:Z:107:ARG:NH1  | 2.28                     | 0.48              |
| 1:2:51:U:H2'     | 1:2:52:G:C8       | 2.49                     | 0.48              |
| 1:2:533:C:H2'    | 1:2:534:G:O4'     | 2.12                     | 0.48              |
| 1:2:1142:C:O2'   | 1:2:1146:A:N1     | 2.43                     | 0.48              |
| 1:2:1584:A:H2'   | 1:2:1585:C:O4'    | 2.14                     | 0.48              |
| 9:J:168:HIS:ND1  | 9:J:169:LYS:HG3   | 2.28                     | 0.48              |
| 10:K:141:ARG:NH2 | 10:K:142:SER:O    | 2.39                     | 0.48              |
| 13:N:78:THR:OG1  | 13:N:87:VAL:O     | 2.27                     | 0.48              |
| 17:R:81:ARG:HB2  | 17:R:117:GLY:HA3  | 1.95                     | 0.48              |
| 1:2:144:U:H2'    | 1:2:145:G:C8      | 2.49                     | 0.48              |
| 1:2:422:G:H2'    | 1:2:423:A:C8      | 2.48                     | 0.48              |
| 1:2:520:U:H2'    | 1:2:521:A:H8      | 1.76                     | 0.48              |
| 1:2:571:U:H2'    | 1:2:572:U:C6      | 2.48                     | 0.48              |
| 1:2:663:G:H2'    | 1:2:664:C:H6      | 1.78                     | 0.48              |
| 1:2:1089:A:H1'   | 24:Y:9:ASP:OD1    | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1232:G:O6     | 20:U:137:LYS:HE3  | 2.14                     | 0.48              |
| 1:2:1837:G:OP2    | 35:l:4:LYS:HG2    | 2.14                     | 0.48              |
| 6:G:35:PRO:HG2    | 6:G:36:HIS:HD1    | 1.78                     | 0.48              |
| 20:U:114:LEU:HA   | 20:U:117:ILE:HB   | 1.94                     | 0.48              |
| 24:Y:59:GLY:C     | 24:Y:60:LYS:HD3   | 2.37                     | 0.48              |
| 25:Z:68:LYS:HZ2   | 34:i:83:VAL:HA    | 1.77                     | 0.48              |
| 25:Z:81:ILE:HG12  | 25:Z:120:PHE:CD2  | 2.49                     | 0.48              |
| 1:2:550:A:H2'     | 1:2:551:A:C8      | 2.48                     | 0.48              |
| 1:2:1027:A:H2'    | 1:2:1028:C:C6     | 2.49                     | 0.48              |
| 1:2:1088:G:C2     | 1:2:1154:G:C6     | 3.02                     | 0.48              |
| 1:2:1274:A:C4     | 1:2:1316:G:N2     | 2.81                     | 0.48              |
| 1:2:1448:A:N6     | 1:2:1469:G:O2'    | 2.47                     | 0.48              |
| 1:2:1561:G:O3'    | 1:2:1562:G:N2     | 2.44                     | 0.48              |
| 6:G:163:ASP:OD1   | 6:G:164:LEU:N     | 2.47                     | 0.48              |
| 16:Q:149:ARG:N    | 27:b:26:CYS:O     | 2.47                     | 0.48              |
| 22:W:66:ARG:HE    | 22:W:77:TRP:CD1   | 2.32                     | 0.48              |
| 34:i:86:VAL:HG12  | 34:i:86:VAL:O     | 2.14                     | 0.48              |
| 36:y:56:G:O2'     | 36:y:57:A:O4'     | 2.27                     | 0.48              |
| 1:2:1290:G:H2'    | 1:2:1291:A:H8     | 1.78                     | 0.48              |
| 1:2:1732:G:O6     | 1:2:1791:U:C2     | 2.66                     | 0.48              |
| 5:F:36:GLY:C      | 5:F:51:LEU:HB3    | 2.39                     | 0.48              |
| 12:M:5:LYS:HA     | 12:M:8:ARG:HH11   | 1.79                     | 0.48              |
| 14:O:52:LEU:HD11  | 14:O:62:VAL:HG12  | 1.96                     | 0.48              |
| 22:W:24:LEU:HD13  | 22:W:32:LEU:HB2   | 1.95                     | 0.48              |
| 32:g:66:VAL:HG22  | 32:g:82:SER:OG    | 2.13                     | 0.48              |
| 1:2:1824:U:OP2    | 37:z:834:A:O2'    | 2.31                     | 0.48              |
| 5:F:1:MET:HG2     | 5:F:4:GLN:HB2     | 1.95                     | 0.48              |
| 5:F:20:GLU:OE2    | 5:F:76:ARG:NE     | 2.47                     | 0.48              |
| 7:H:38:TYR:OH     | 29:d:51:ARG:NH1   | 2.37                     | 0.48              |
| 7:H:124:ASP:OD1   | 7:H:125:SER:N     | 2.46                     | 0.48              |
| 19:T:36:GLU:HB3   | 19:T:47:ARG:HD2   | 1.96                     | 0.48              |
| 25:Z:1:MET:HE3    | 25:Z:5:ARG:HE     | 1.79                     | 0.48              |
| 32:g:270:LEU:HD21 | 32:g:298:LEU:HD11 | 1.96                     | 0.48              |
| 37:z:527:G:H2'    | 37:z:528:C:C6     | 2.48                     | 0.48              |
| 1:2:121:U:H5''    | 6:G:77:ARG:NH1    | 2.29                     | 0.48              |
| 1:2:411:G:OP1     | 13:N:97:ARG:NH1   | 2.47                     | 0.48              |
| 1:2:446:C:O2      | 1:2:1794:A:O2'    | 2.32                     | 0.48              |
| 1:2:497:G:OP2     | 26:a:104:ARG:NH2  | 2.47                     | 0.48              |
| 1:2:878:U:H2'     | 1:2:879:U:C6      | 2.49                     | 0.48              |
| 1:2:1007:A:OP1    | 15:P:3:ARG:NH1    | 2.46                     | 0.48              |
| 1:2:1344:G:N2     | 1:2:1377:G:H22    | 2.12                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:59:ASP:O      | 6:G:62:LYS:HG3    | 2.13                     | 0.48              |
| 9:J:144:ILE:HD11  | 24:Y:52:ILE:HG22  | 1.96                     | 0.48              |
| 10:K:190:LEU:HD23 | 10:K:195:LEU:HD23 | 1.95                     | 0.48              |
| 17:R:98:ASN:HB3   | 17:R:120:SER:HB2  | 1.95                     | 0.48              |
| 18:S:10:VAL:HG21  | 18:S:98:LYS:HZ3   | 1.77                     | 0.48              |
| 23:X:40:ASP:OD2   | 23:X:43:THR:OG1   | 2.26                     | 0.48              |
| 32:g:41:ILE:HG21  | 32:g:55:PRO:HB3   | 1.96                     | 0.48              |
| 36:y:60:C:H2'     | 36:y:61:C:C6      | 2.49                     | 0.48              |
| 1:2:106:C:H5''    | 1:2:421:G:O2'     | 2.13                     | 0.47              |
| 1:2:603:C:OP1     | 34:i:75:LYS:N     | 2.47                     | 0.47              |
| 1:2:1347:G:H2'    | 1:2:1348:G:C8     | 2.44                     | 0.47              |
| 1:2:1528:A:N6     | 1:2:1529:C:H41    | 2.12                     | 0.47              |
| 1:2:1629:A:H2'    | 1:2:1630:C:O4'    | 2.13                     | 0.47              |
| 1:2:1863:A:C6     | 3:D:115:LYS:HG2   | 2.48                     | 0.47              |
| 10:K:38:ILE:HD12  | 10:K:60:LEU:O     | 2.13                     | 0.47              |
| 10:K:89:GLU:OE1   | 10:K:92:ARG:NH1   | 2.47                     | 0.47              |
| 15:P:83:ASP:OD1   | 15:P:84:LEU:HD23  | 2.13                     | 0.47              |
| 28:c:16:LYS:HA    | 28:c:23:ARG:HD2   | 1.95                     | 0.47              |
| 32:g:17:TRP:HB2   | 32:g:36:ARG:HD2   | 1.96                     | 0.47              |
| 32:g:22:ALA:HB3   | 32:g:32:LEU:HB2   | 1.96                     | 0.47              |
| 1:2:343:C:H2'     | 1:2:344:U:C6      | 2.48                     | 0.47              |
| 1:2:678:U:H5      | 1:2:736:C:H42     | 1.61                     | 0.47              |
| 1:2:1125:G:H2'    | 1:2:1126:G:N9     | 2.30                     | 0.47              |
| 1:2:1551:A:H3'    | 30:e:13:LYS:HE2   | 1.96                     | 0.47              |
| 1:2:1554:C:H2'    | 1:2:1555:U:O4'    | 2.13                     | 0.47              |
| 1:2:1601:G:N2     | 1:2:1627:G:O2'    | 2.44                     | 0.47              |
| 2:C:189:ILE:H     | 2:C:189:ILE:HD12  | 1.78                     | 0.47              |
| 5:F:196:GLY:C     | 5:F:198:ILE:HA    | 2.39                     | 0.47              |
| 6:G:137:PRO:HB2   | 6:G:150:PRO:HD2   | 1.95                     | 0.47              |
| 16:Q:26:ASN:HB3   | 16:Q:92:ALA:HB2   | 1.96                     | 0.47              |
| 16:Q:132:VAL:HG13 | 16:Q:132:VAL:O    | 2.14                     | 0.47              |
| 18:S:38:PRO:HG2   | 21:V:8:ASP:HA     | 1.96                     | 0.47              |
| 18:S:105:LYS:HA   | 18:S:108:ILE:HG22 | 1.96                     | 0.47              |
| 20:U:123:LEU:HB3  | 20:U:127:TRP:HZ3  | 1.78                     | 0.47              |
| 28:c:32:PHE:HA    | 28:c:47:PHE:HA    | 1.95                     | 0.47              |
| 28:c:34:ASP:HA    | 28:c:45:THR:HA    | 1.94                     | 0.47              |
| 32:g:101:PHE:HB3  | 32:g:132:TRP:CZ3  | 2.49                     | 0.47              |
| 37:z:534:A:O2'    | 37:z:535:A:O5'    | 2.30                     | 0.47              |
| 37:z:837:G:H4'    | 37:z:838:C:H5'    | 1.95                     | 0.47              |
| 1:2:89:C:H2'      | 1:2:90:G:C8       | 2.50                     | 0.47              |
| 1:2:477:U:O4'     | 1:2:503:G:N2      | 2.47                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:744:C:H2'     | 1:2:745:U:C2      | 2.48                     | 0.47              |
| 1:2:942:U:H2'     | 1:2:943:G:H8      | 1.79                     | 0.47              |
| 1:2:1411:C:H2'    | 1:2:1412:C:C6     | 2.49                     | 0.47              |
| 1:2:1833:U:H5'    | 16:Q:150:ARG:NH1  | 2.30                     | 0.47              |
| 4:E:69:PHE:CD2    | 4:E:71:LEU:HB2    | 2.48                     | 0.47              |
| 7:H:133:THR:OG1   | 7:H:135:ARG:NH1   | 2.47                     | 0.47              |
| 8:I:202:ASN:OD1   | 8:I:203:LYS:N     | 2.47                     | 0.47              |
| 11:L:134:HIS:HE1  | 11:L:164:PRO:HD2  | 1.78                     | 0.47              |
| 25:Z:100:VAL:HG12 | 25:Z:125:VAL:HG12 | 1.96                     | 0.47              |
| 30:e:22:ARG:HB2   | 30:e:38:MET:HE1   | 1.95                     | 0.47              |
| 33:h:80:ARG:HD3   | 33:h:81:GLY:H     | 1.79                     | 0.47              |
| 1:2:909:A:N6      | 9:J:98:ARG:HD2    | 2.30                     | 0.47              |
| 1:2:917:G:H2'     | 24:Y:28:ARG:NH2   | 2.29                     | 0.47              |
| 1:2:957:G:C2      | 37:z:831:A:N1     | 2.83                     | 0.47              |
| 1:2:1033:G:H2'    | 1:2:1034:U:H6     | 1.79                     | 0.47              |
| 1:2:1609:A:OP2    | 17:R:42:ARG:NH2   | 2.47                     | 0.47              |
| 7:H:20:PHE:HD2    | 7:H:23:TRP:HD1    | 1.62                     | 0.47              |
| 11:L:170:PRO:O    | 11:L:175:ARG:NH2  | 2.41                     | 0.47              |
| 23:X:38:GLU:OE1   | 23:X:50:SER:HA    | 2.14                     | 0.47              |
| 37:z:540:C:H2'    | 37:z:541:C:C6     | 2.49                     | 0.47              |
| 37:z:579:G:H2'    | 37:z:580:U:H6     | 1.79                     | 0.47              |
| 1:2:151:C:H2'     | 1:2:152:U:C6      | 2.49                     | 0.47              |
| 1:2:279:G:H1'     | 6:G:131:VAL:HG21  | 1.96                     | 0.47              |
| 1:2:324:C:OP2     | 8:I:190:ARG:NH2   | 2.47                     | 0.47              |
| 1:2:526:A:H62     | 1:2:537:G:N2      | 2.13                     | 0.47              |
| 1:2:951:A:H4'     | 1:2:952:G:H4'     | 1.97                     | 0.47              |
| 1:2:1031:A:H2'    | 1:2:1032:A:O4'    | 2.15                     | 0.47              |
| 1:2:1257:C:O2     | 30:e:10:HIS:NE2   | 2.47                     | 0.47              |
| 1:2:1332:C:H2'    | 1:2:1333:C:O4'    | 2.14                     | 0.47              |
| 1:2:1405:A:OP1    | 18:S:26:LYS:NZ    | 2.45                     | 0.47              |
| 4:E:249:SER:HB2   | 4:E:252:GLN:HE22  | 1.78                     | 0.47              |
| 7:H:174:ALA:O     | 7:H:178:ILE:HG12  | 2.14                     | 0.47              |
| 8:I:7:PHE:CE2     | 8:I:9:ALA:HB3     | 2.49                     | 0.47              |
| 11:L:95:ASP:OD1   | 11:L:96:TYR:N     | 2.47                     | 0.47              |
| 15:P:23:PRO:HB2   | 15:P:25:TRP:CE3   | 2.49                     | 0.47              |
| 18:S:146:ARG:NE   | 36:y:31:C:OP2     | 2.39                     | 0.47              |
| 22:W:19:ARG:O     | 22:W:118:ASP:N    | 2.48                     | 0.47              |
| 32:g:174:VAL:HB   | 32:g:188:HIS:ND1  | 2.30                     | 0.47              |
| 1:2:522:C:H2'     | 1:2:523:A:H8      | 1.79                     | 0.47              |
| 1:2:871:A:H2'     | 1:2:872:C:C6      | 2.49                     | 0.47              |
| 1:2:908:C:H3'     | 1:2:909:A:H3'     | 1.96                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:1093:G:H2'   | 1:2:1094:C:C6     | 2.50                     | 0.47              |
| 1:2:1142:C:H2'   | 1:2:1143:C:C6     | 2.50                     | 0.47              |
| 1:2:1847:C:H5    | 35:l:5:TRP:CZ3    | 2.33                     | 0.47              |
| 4:E:249:SER:HB2  | 4:E:252:GLN:NE2   | 2.30                     | 0.47              |
| 9:J:146:VAL:HB   | 24:Y:49:GLU:OE1   | 2.14                     | 0.47              |
| 26:a:15:ASN:ND2  | 26:a:22:GLN:OE1   | 2.47                     | 0.47              |
| 1:2:18:C:O3'     | 25:Z:107:ARG:NH1  | 2.48                     | 0.47              |
| 1:2:337:G:H2'    | 1:2:338:A:C8      | 2.50                     | 0.47              |
| 1:2:361:A:OP2    | 10:K:10:LYS:HG3   | 2.15                     | 0.47              |
| 1:2:514:U:H5'    | 1:2:515:A:H5'     | 1.96                     | 0.47              |
| 1:2:525:G:H2'    | 1:2:526:A:H8      | 1.80                     | 0.47              |
| 1:2:542:G:H4'    | 34:i:114:ARG:HD3  | 1.96                     | 0.47              |
| 1:2:553:G:N7     | 1:2:576:G:N2      | 2.62                     | 0.47              |
| 1:2:965:U:H3'    | 1:2:966:G:N2      | 2.28                     | 0.47              |
| 1:2:999:U:H5''   | 3:D:165:ARG:NH1   | 2.29                     | 0.47              |
| 1:2:1125:G:H2'   | 1:2:1126:G:C4     | 2.50                     | 0.47              |
| 1:2:1373:U:H3'   | 2:C:102:ARG:NH2   | 2.29                     | 0.47              |
| 1:2:1398:A:H2'   | 1:2:1401:A:C5     | 2.49                     | 0.47              |
| 1:2:1402:G:H2'   | 1:2:1403:U:C6     | 2.49                     | 0.47              |
| 2:C:85:ARG:HH21  | 19:T:82:ASP:C     | 2.22                     | 0.47              |
| 5:F:53:THR:O     | 5:F:90:LYS:HG3    | 2.15                     | 0.47              |
| 5:F:100:ALA:O    | 5:F:104:SER:N     | 2.41                     | 0.47              |
| 6:G:255:ARG:NH1  | 6:G:255:ARG:O     | 2.48                     | 0.47              |
| 7:H:77:MET:SD    | 7:H:84:GLY:N      | 2.88                     | 0.47              |
| 8:I:216:ARG:O    | 8:I:218:LYS:N     | 2.48                     | 0.47              |
| 9:J:126:HIS:O    | 9:J:130:LEU:HD23  | 2.15                     | 0.47              |
| 11:L:26:ASP:OD1  | 34:i:115:ARG:NH2  | 2.47                     | 0.47              |
| 11:L:136:ARG:HG2 | 11:L:141:VAL:HG22 | 1.96                     | 0.47              |
| 11:L:176:LYS:O   | 11:L:180:LYS:HG2  | 2.15                     | 0.47              |
| 15:P:5:HIS:HD2   | 15:P:121:ARG:HE   | 1.63                     | 0.47              |
| 18:S:132:PHE:O   | 18:S:140:ARG:NH1  | 2.36                     | 0.47              |
| 27:b:52:ASP:HA   | 27:b:55:GLU:HG2   | 1.96                     | 0.47              |
| 32:g:208:ALA:HA  | 32:g:218:LEU:HD13 | 1.96                     | 0.47              |
| 37:z:584:A:H2'   | 37:z:586:A:N7     | 2.30                     | 0.47              |
| 1:2:12:U:H2'     | 1:2:13:C:C6       | 2.50                     | 0.47              |
| 1:2:91:A:P       | 1:2:436:G:H22     | 2.37                     | 0.47              |
| 1:2:318:U:H2'    | 1:2:319:G:H8      | 1.80                     | 0.47              |
| 1:2:443:C:H2'    | 1:2:444:U:H6      | 1.79                     | 0.47              |
| 1:2:837:G:H2'    | 1:2:838:C:C6      | 2.50                     | 0.47              |
| 1:2:921:G:O2'    | 15:P:87:ASP:OD1   | 2.32                     | 0.47              |
| 1:2:1053:C:H5'   | 37:z:832:A:H4'    | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:1090:C:O2    | 24:Y:16:ASN:ND2  | 2.48                     | 0.47              |
| 1:2:1748:G:H2'   | 1:2:1749:C:H6    | 1.80                     | 0.47              |
| 2:C:76:VAL:HA    | 2:C:123:VAL:HB   | 1.96                     | 0.47              |
| 3:D:185:VAL:HA   | 3:D:188:LEU:HG   | 1.97                     | 0.47              |
| 8:I:102:VAL:HG22 | 8:I:106:LEU:HD11 | 1.97                     | 0.47              |
| 10:K:8:TRP:O     | 10:K:18:ARG:HD2  | 2.15                     | 0.47              |
| 19:T:13:ALA:O    | 19:T:17:ILE:HG22 | 2.14                     | 0.47              |
| 24:Y:87:GLU:HA   | 24:Y:90:GLN:HG3  | 1.96                     | 0.47              |
| 26:a:39:GLU:O    | 26:a:43:LYS:HG2  | 2.14                     | 0.47              |
| 28:c:34:ASP:HB2  | 28:c:82:LYS:HE2  | 1.96                     | 0.47              |
| 33:h:91:LEU:HD23 | 33:h:94:LYS:HD2  | 1.97                     | 0.47              |
| 36:y:34:A:H2'    | 36:y:35:U:C6     | 2.50                     | 0.47              |
| 1:2:146:G:O2'    | 1:2:147:A:H8     | 1.98                     | 0.47              |
| 1:2:413:U:H2'    | 1:2:414:C:H6     | 1.79                     | 0.47              |
| 1:2:425:A:OP1    | 10:K:23:LYS:NZ   | 2.28                     | 0.47              |
| 1:2:1007:A:H5''  | 15:P:3:ARG:HH12  | 1.80                     | 0.47              |
| 1:2:1199:G:H2'   | 1:2:1200:A:H8    | 1.80                     | 0.47              |
| 1:2:1319:U:H2'   | 1:2:1320:G:C8    | 2.49                     | 0.47              |
| 1:2:1443:G:H2'   | 1:2:1444:A:C8    | 2.50                     | 0.47              |
| 1:2:1702:U:H2'   | 1:2:1703:C:C6    | 2.49                     | 0.47              |
| 1:2:1789:G:H2'   | 1:2:1790:G:H8    | 1.79                     | 0.47              |
| 2:C:85:ARG:HB2   | 2:C:205:ARG:NH1  | 2.30                     | 0.47              |
| 4:E:133:ALA:O    | 4:E:136:ILE:HG22 | 2.14                     | 0.47              |
| 8:I:199:THR:HA   | 8:I:202:ASN:ND2  | 2.29                     | 0.47              |
| 9:J:160:LYS:HA   | 9:J:189:PHE:CZ   | 2.49                     | 0.47              |
| 1:2:1002:C:H2'   | 1:2:1003:C:C6    | 2.50                     | 0.47              |
| 1:2:1191:A:H2'   | 1:2:1192:A:C8    | 2.50                     | 0.47              |
| 1:2:1196:A:H2'   | 1:2:1197:U:C6    | 2.50                     | 0.47              |
| 1:2:1612:G:H1    | 17:R:40:ARG:NH2  | 2.13                     | 0.47              |
| 1:2:1798:U:H2'   | 1:2:1799:G:H8    | 1.80                     | 0.47              |
| 1:2:1832:U:O2'   | 16:Q:150:ARG:NH2 | 2.43                     | 0.47              |
| 6:G:6:LYS:HB3    | 6:G:30:ARG:HH22  | 1.79                     | 0.47              |
| 11:L:89:GLU:HA   | 11:L:92:MET:HG2  | 1.97                     | 0.47              |
| 22:W:50:VAL:HG23 | 22:W:91:LEU:HG   | 1.97                     | 0.47              |
| 26:a:20:ARG:HH11 | 26:a:76:TYR:HH   | 1.59                     | 0.47              |
| 1:2:203:G:H2'    | 1:2:204:G:O4'    | 2.14                     | 0.46              |
| 1:2:215:U:H2'    | 1:2:216:U:H6     | 1.80                     | 0.46              |
| 1:2:284:C:H2'    | 1:2:286:C:H5'    | 1.97                     | 0.46              |
| 1:2:1091:U:O2'   | 24:Y:20:ARG:NH1  | 2.48                     | 0.46              |
| 1:2:1270:G:OP1   | 1:2:1270:G:N2    | 2.30                     | 0.46              |
| 1:2:1509:G:H2'   | 1:2:1510:G:H8    | 1.80                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:G:89:VAL:HG12  | 6:G:100:ARG:HG3   | 1.96                     | 0.46              |
| 8:I:76:LEU:HD23  | 8:I:94:ARG:HB2    | 1.97                     | 0.46              |
| 13:N:49:GLU:HB2  | 13:N:116:CYS:SG   | 2.55                     | 0.46              |
| 36:y:30:G:H2'    | 36:y:31:C:C6      | 2.50                     | 0.46              |
| 36:y:30:G:H2'    | 36:y:31:C:H6      | 1.80                     | 0.46              |
| 1:2:317:G:H1'    | 1:2:318:U:C6      | 2.50                     | 0.46              |
| 1:2:820:C:H5'    | 11:L:147:PHE:CE1  | 2.50                     | 0.46              |
| 1:2:1034:U:H1'   | 1:2:1176:C:H42    | 1.81                     | 0.46              |
| 1:2:1289:A:H2'   | 1:2:1290:G:H8     | 1.79                     | 0.46              |
| 1:2:1413:C:C2    | 1:2:1415:C:C5     | 3.04                     | 0.46              |
| 1:2:1615:A:P     | 17:R:40:ARG:HH21  | 2.38                     | 0.46              |
| 1:2:1652:G:H2'   | 1:2:1653:G:H8     | 1.81                     | 0.46              |
| 1:2:1804:U:H2'   | 1:2:1805:C:C6     | 2.49                     | 0.46              |
| 7:H:78:MET:HG3   | 7:H:159:ARG:NH1   | 2.30                     | 0.46              |
| 9:J:69:LEU:HA    | 9:J:72:PHE:CD1    | 2.51                     | 0.46              |
| 10:K:12:ARG:HG2  | 10:K:13:LYS:N     | 2.29                     | 0.46              |
| 13:N:61:PRO:HB3  | 13:N:68:ILE:HD11  | 1.97                     | 0.46              |
| 15:P:63:VAL:HG21 | 15:P:71:ILE:HD11  | 1.96                     | 0.46              |
| 18:S:22:VAL:HB   | 18:S:71:ARG:HG3   | 1.97                     | 0.46              |
| 19:T:93:GLN:HG3  | 19:T:95:ILE:HG22  | 1.98                     | 0.46              |
| 27:b:21:ILE:N    | 27:b:30:VAL:O     | 2.34                     | 0.46              |
| 1:2:17:C:H2'     | 1:2:18:C:C6       | 2.50                     | 0.46              |
| 1:2:551:A:N7     | 11:L:173:VAL:HG21 | 2.30                     | 0.46              |
| 1:2:903:G:H2'    | 1:2:904:A:H8      | 1.81                     | 0.46              |
| 1:2:1748:G:H2'   | 1:2:1749:C:C6     | 2.50                     | 0.46              |
| 6:G:54:TYR:HE2   | 26:a:17:LEU:HB3   | 1.80                     | 0.46              |
| 21:V:75:MET:O    | 21:V:78:ILE:HG22  | 2.15                     | 0.46              |
| 22:W:94:PRO:HD2  | 22:W:97:ILE:HD11  | 1.96                     | 0.46              |
| 24:Y:52:ILE:HD12 | 24:Y:60:LYS:C     | 2.40                     | 0.46              |
| 36:y:68:U:H2'    | 36:y:69:G:C8      | 2.51                     | 0.46              |
| 1:2:185:C:H2'    | 1:2:186:G:C8      | 2.50                     | 0.46              |
| 1:2:444:U:H2'    | 1:2:445:A:C8      | 2.50                     | 0.46              |
| 1:2:728:U:H5''   | 1:2:729:C:C6      | 2.50                     | 0.46              |
| 1:2:840:U:H2'    | 1:2:841:G:C8      | 2.50                     | 0.46              |
| 1:2:910:U:O2'    | 9:J:120:ARG:NH2   | 2.48                     | 0.46              |
| 1:2:1108:U:H3    | 1:2:1109:A:H62    | 1.62                     | 0.46              |
| 1:2:1160:G:H2'   | 1:2:1161:G:C2     | 2.50                     | 0.46              |
| 2:C:68:ILE:HD11  | 2:C:121:LEU:HG    | 1.96                     | 0.46              |
| 10:K:199:LEU:HA  | 10:K:202:ILE:HG12 | 1.97                     | 0.46              |
| 11:L:108:ARG:HE  | 11:L:154:GLN:HE22 | 1.62                     | 0.46              |
| 15:P:75:LEU:HB3  | 15:P:81:ALA:HA    | 1.96                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 27:b:49:ALA:O     | 27:b:53:ILE:HB   | 2.15                     | 0.46              |
| 1:2:73:C:O2       | 1:2:74:G:H1'     | 2.16                     | 0.46              |
| 1:2:294:C:H2'     | 1:2:295:C:C6     | 2.50                     | 0.46              |
| 1:2:483:A:H62     | 1:2:499:G:N2     | 2.12                     | 0.46              |
| 1:2:1103:G:C6     | 1:2:1122:G:C6    | 3.04                     | 0.46              |
| 1:2:1214:C:H2'    | 1:2:1215:C:C6    | 2.51                     | 0.46              |
| 1:2:1333:C:HO2'   | 22:W:68:THR:HG1  | 1.53                     | 0.46              |
| 1:2:1701:G:H4'    | 35:l:2:ARG:HH12  | 1.81                     | 0.46              |
| 2:C:57:LYS:HE2    | 2:C:159:ILE:HD11 | 1.97                     | 0.46              |
| 2:C:70:ASN:ND2    | 4:E:259:VAL:HG21 | 2.30                     | 0.46              |
| 3:D:145:LYS:NZ    | 3:D:149:GLN:O    | 2.48                     | 0.46              |
| 8:I:55:GLY:H      | 8:I:63:MET:HB2   | 1.81                     | 0.46              |
| 9:J:51:ILE:HG12   | 9:J:61:ILE:HD11  | 1.98                     | 0.46              |
| 9:J:78:ARG:HH12   | 9:J:81:ARG:HD2   | 1.80                     | 0.46              |
| 10:K:103:LEU:HD22 | 10:K:170:LYS:HB3 | 1.97                     | 0.46              |
| 15:P:19:ARG:HD2   | 15:P:21:SER:HB2  | 1.98                     | 0.46              |
| 25:Z:68:LYS:NZ    | 34:i:83:VAL:HA   | 2.31                     | 0.46              |
| 28:c:19:HIS:HB3   | 28:c:22:LYS:NZ   | 2.30                     | 0.46              |
| 28:c:67:THR:OG1   | 28:c:70:LYS:O    | 2.28                     | 0.46              |
| 32:g:31:ILE:HG22  | 32:g:43:TRP:HB2  | 1.98                     | 0.46              |
| 34:i:102:ARG:HH11 | 34:i:106:ALA:HB1 | 1.80                     | 0.46              |
| 36:y:67:C:H2'     | 36:y:68:U:C6     | 2.51                     | 0.46              |
| 37:z:560:C:H2'    | 37:z:561:U:C6    | 2.50                     | 0.46              |
| 1:2:297:C:H2'     | 1:2:298:G:C8     | 2.51                     | 0.46              |
| 1:2:330:C:H2'     | 1:2:331:C:C6     | 2.51                     | 0.46              |
| 1:2:950:U:P       | 3:D:24:PRO:HG3   | 2.55                     | 0.46              |
| 1:2:1002:C:H2'    | 1:2:1003:C:H6    | 1.80                     | 0.46              |
| 1:2:1088:G:C2     | 1:2:1089:A:N7    | 2.84                     | 0.46              |
| 1:2:1571:G:H2'    | 1:2:1572:G:H8    | 1.79                     | 0.46              |
| 5:F:140:GLY:HA3   | 5:F:182:LEU:HD23 | 1.98                     | 0.46              |
| 7:H:39:ILE:HG23   | 7:H:68:ILE:HG13  | 1.97                     | 0.46              |
| 9:J:116:ARG:NH2   | 9:J:121:THR:OG1  | 2.49                     | 0.46              |
| 15:P:27:LYS:HG3   | 15:P:28:LEU:HG   | 1.97                     | 0.46              |
| 26:a:20:ARG:NH1   | 26:a:76:TYR:OH   | 2.40                     | 0.46              |
| 32:g:60:ARG:O     | 32:g:90:TRP:HH2  | 1.98                     | 0.46              |
| 33:h:62:VAL:HG22  | 33:h:97:ILE:HD11 | 1.97                     | 0.46              |
| 1:2:370:G:H1'     | 10:K:5:ARG:NE    | 2.30                     | 0.46              |
| 1:2:678:U:O2'     | 1:2:679:U:OP2    | 2.31                     | 0.46              |
| 1:2:1672:U:OP2    | 7:H:63:LYS:NZ    | 2.48                     | 0.46              |
| 1:2:1741:U:OP1    | 8:I:31:ARG:NH2   | 2.49                     | 0.46              |
| 2:C:178:LEU:HD12  | 2:C:178:LEU:HA   | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:193:ILE:H     | 3:D:193:ILE:HD12  | 1.80                     | 0.46              |
| 4:E:45:TRP:HZ3    | 4:E:56:LYS:HD3    | 1.81                     | 0.46              |
| 6:G:202:PRO:HB2   | 13:N:42:LEU:HD13  | 1.98                     | 0.46              |
| 7:H:35:LEU:HD12   | 7:H:117:ILE:HD12  | 1.98                     | 0.46              |
| 21:V:14:PHE:CZ    | 21:V:18:LEU:HD22  | 2.51                     | 0.46              |
| 27:b:12:LYS:NZ    | 27:b:33:ASP:O     | 2.49                     | 0.46              |
| 32:g:172:LYS:HG2  | 32:g:194:TYR:HA   | 1.96                     | 0.46              |
| 37:z:569:A:H2'    | 37:z:570:A:O4'    | 2.15                     | 0.46              |
| 1:2:976:A:H2'     | 1:2:977:A:C8      | 2.51                     | 0.46              |
| 1:2:1262:C:C4     | 1:2:1512:G:N2     | 2.84                     | 0.46              |
| 1:2:1322:U:O4     | 30:e:28:HIS:NE2   | 2.46                     | 0.46              |
| 1:2:1545:G:H3'    | 1:2:1574:A:H61    | 1.81                     | 0.46              |
| 2:C:19:LEU:HD11   | 19:T:106:LEU:HD11 | 1.98                     | 0.46              |
| 2:C:35:GLU:O      | 2:C:38:ILE:HG22   | 2.16                     | 0.46              |
| 2:C:151:ASP:N     | 2:C:151:ASP:OD1   | 2.47                     | 0.46              |
| 3:D:89:GLU:N      | 3:D:89:GLU:OE1    | 2.48                     | 0.46              |
| 4:E:163:HIS:CG    | 4:E:185:ARG:HG2   | 2.51                     | 0.46              |
| 15:P:113:PHE:CE2  | 15:P:117:LEU:HD11 | 2.50                     | 0.46              |
| 23:X:19:ALA:HB2   | 23:X:55:ILE:HD12  | 1.98                     | 0.46              |
| 30:e:40:ARG:NH1   | 30:e:41:GLN:HG3   | 2.30                     | 0.46              |
| 30:e:52:PHE:O     | 30:e:53:ILE:HD13  | 2.16                     | 0.46              |
| 1:2:76:U:OP2      | 8:I:159:ARG:NH1   | 2.49                     | 0.46              |
| 1:2:524:G:H2'     | 1:2:525:G:C8      | 2.50                     | 0.46              |
| 1:2:869:G:O2'     | 1:2:870:G:H8      | 1.97                     | 0.46              |
| 2:C:169:HIS:HB3   | 2:C:203:PHE:CE1   | 2.51                     | 0.46              |
| 3:D:40:ASN:H      | 3:D:75:GLN:NE2    | 2.12                     | 0.46              |
| 5:F:227:LYS:HZ1   | 32:g:187:ASN:CG   | 2.23                     | 0.46              |
| 15:P:45:LEU:HB3   | 15:P:49:GLN:HB2   | 1.98                     | 0.46              |
| 21:V:44:GLU:OE1   | 21:V:44:GLU:N     | 2.48                     | 0.46              |
| 22:W:67:LYS:HA    | 30:e:44:ARG:NH1   | 2.31                     | 0.46              |
| 23:X:21:ASN:ND2   | 24:Y:66:THR:HB    | 2.31                     | 0.46              |
| 36:y:65:C:H2'     | 36:y:66:U:C6      | 2.51                     | 0.46              |
| 1:2:1276:G:N2     | 1:2:1313:U:H3     | 2.14                     | 0.46              |
| 1:2:1795:A:H2'    | 1:2:1796:C:C6     | 2.51                     | 0.46              |
| 3:D:107:ARG:HH22  | 16:Q:131:ASP:C    | 2.24                     | 0.46              |
| 7:H:145:ARG:HA    | 7:H:148:ASN:ND2   | 2.31                     | 0.46              |
| 11:L:85:GLY:HA3   | 11:L:151:LEU:HD13 | 1.97                     | 0.46              |
| 11:L:109:ARG:NE   | 11:L:111:GLN:HE22 | 2.14                     | 0.46              |
| 28:c:79:PHE:O     | 28:c:80:ARG:NH1   | 2.40                     | 0.46              |
| 32:g:154:VAL:HG13 | 32:g:166:VAL:O    | 2.16                     | 0.46              |
| 1:2:64:A:H2       | 1:2:83:A:H62      | 1.63                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:168:C:H4'    | 8:I:131:ARG:HH21  | 1.81                     | 0.45              |
| 1:2:220:C:H2'    | 1:2:221:A:H8      | 1.81                     | 0.45              |
| 1:2:540:C:H2'    | 1:2:541:U:C6      | 2.51                     | 0.45              |
| 1:2:957:G:H2'    | 1:2:958:A:C8      | 2.52                     | 0.45              |
| 1:2:1007:A:H5''  | 15:P:3:ARG:NH2    | 2.31                     | 0.45              |
| 1:2:1138:G:H2'   | 1:2:1140:A:OP2    | 2.16                     | 0.45              |
| 1:2:1222:G:N2    | 1:2:1634:G:C8     | 2.84                     | 0.45              |
| 2:C:8:LEU:HD11   | 23:X:39:VAL:HG21  | 1.99                     | 0.45              |
| 6:G:64:ILE:HD12  | 26:a:17:LEU:HG    | 1.98                     | 0.45              |
| 8:I:161:PRO:HA   | 8:I:171:THR:HA    | 1.98                     | 0.45              |
| 8:I:232:ARG:O    | 8:I:236:SER:OG    | 2.28                     | 0.45              |
| 10:K:81:VAL:HG12 | 10:K:102:VAL:HG12 | 1.97                     | 0.45              |
| 11:L:24:ARG:HH21 | 11:L:25:LEU:HD21  | 1.81                     | 0.45              |
| 11:L:128:VAL:O   | 11:L:132:GLN:HB2  | 2.16                     | 0.45              |
| 14:O:26:LEU:HD12 | 14:O:31:LEU:HD21  | 1.97                     | 0.45              |
| 22:W:40:ILE:O    | 22:W:44:LYS:HG2   | 2.15                     | 0.45              |
| 36:y:52:G:H21    | 36:y:53:A:H62     | 1.64                     | 0.45              |
| 1:2:36:U:H2'     | 1:2:37:C:H6       | 1.81                     | 0.45              |
| 1:2:149:A:N7     | 1:2:169:U:C4      | 2.84                     | 0.45              |
| 1:2:664:C:H2'    | 1:2:665:U:H6      | 1.80                     | 0.45              |
| 1:2:941:U:H2'    | 1:2:942:U:H6      | 1.79                     | 0.45              |
| 1:2:1019:A:H2'   | 1:2:1020:A:H8     | 1.79                     | 0.45              |
| 1:2:1030:A:H2'   | 1:2:1031:A:O4'    | 2.16                     | 0.45              |
| 1:2:1801:C:H2'   | 1:2:1802:U:O4'    | 2.16                     | 0.45              |
| 3:D:167:LYS:HA   | 3:D:170:GLU:OE1   | 2.17                     | 0.45              |
| 3:D:194:GLY:HA2  | 3:D:197:ILE:HD12  | 1.98                     | 0.45              |
| 4:E:64:GLU:HB2   | 23:X:12:TYR:CD1   | 2.51                     | 0.45              |
| 7:H:140:ASP:HB3  | 29:d:46:VAL:HG22  | 1.97                     | 0.45              |
| 19:T:71:ILE:HG23 | 19:T:74:GLN:H     | 1.81                     | 0.45              |
| 23:X:71:ARG:HH12 | 24:Y:23:ARG:NH1   | 2.15                     | 0.45              |
| 24:Y:4:MET:N     | 24:Y:4:MET:SD     | 2.89                     | 0.45              |
| 1:2:1093:G:H4'   | 2:C:32:PHE:CD1    | 2.52                     | 0.45              |
| 1:2:1105:C:H6    | 19:T:122:PRO:HB3  | 1.81                     | 0.45              |
| 1:2:1273:C:H2'   | 1:2:1274:A:C8     | 2.48                     | 0.45              |
| 1:2:1419:C:O2'   | 1:2:1420:G:O5'    | 2.29                     | 0.45              |
| 2:C:122:LEU:CD1  | 2:C:124:VAL:HG23  | 2.44                     | 0.45              |
| 3:D:62:LEU:O     | 3:D:65:ARG:HG3    | 2.16                     | 0.45              |
| 3:D:217:MET:SD   | 3:D:218:LEU:N     | 2.89                     | 0.45              |
| 9:J:160:LYS:HD2  | 9:J:189:PHE:HZ    | 1.81                     | 0.45              |
| 14:O:20:GLU:HA   | 14:O:23:LYS:HG3   | 1.98                     | 0.45              |
| 14:O:61:TYR:OH   | 14:O:107:SER:HB2  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 20:U:120:HIS:CE1 | 20:U:124:ARG:HD3  | 2.51                     | 0.45              |
| 32:g:296:GLN:HG2 | 32:g:297:THR:HG23 | 1.99                     | 0.45              |
| 36:y:36:A:H3'    | 36:y:37:A:H8      | 1.81                     | 0.45              |
| 36:y:71:U:H3'    | 36:y:73:C:OP2     | 2.16                     | 0.45              |
| 1:2:50:A:OP2     | 1:2:462:C:N4      | 2.49                     | 0.45              |
| 1:2:364:G:O6     | 1:2:375:G:O6      | 2.35                     | 0.45              |
| 1:2:433:U:H2'    | 1:2:434:G:C8      | 2.51                     | 0.45              |
| 1:2:571:U:H1'    | 26:a:33:ALA:HB3   | 1.99                     | 0.45              |
| 1:2:745:U:H2'    | 1:2:746:C:N1      | 2.31                     | 0.45              |
| 1:2:1279:C:H4'   | 31:f:99:LYS:HZ2   | 1.80                     | 0.45              |
| 1:2:1313:U:H2'   | 1:2:1314:G:H8     | 1.80                     | 0.45              |
| 1:2:1324:G:H2'   | 1:2:1325:U:C6     | 2.51                     | 0.45              |
| 1:2:1365:A:H62   | 19:T:3:ARG:H      | 1.62                     | 0.45              |
| 1:2:1460:C:H2'   | 1:2:1461:A:C8     | 2.52                     | 0.45              |
| 1:2:1768:C:H2'   | 1:2:1769:U:H6     | 1.81                     | 0.45              |
| 1:2:1800:A:H2'   | 1:2:1801:C:H6     | 1.79                     | 0.45              |
| 2:C:10:MET:HG3   | 19:T:111:PHE:CE2  | 2.50                     | 0.45              |
| 2:C:26:GLY:H     | 2:C:46:ILE:HG23   | 1.80                     | 0.45              |
| 7:H:78:MET:HG3   | 7:H:159:ARG:HH11  | 1.82                     | 0.45              |
| 9:J:69:LEU:O     | 9:J:73:GLN:HG2    | 2.16                     | 0.45              |
| 11:L:150:ARG:O   | 11:L:154:GLN:HG3  | 2.17                     | 0.45              |
| 19:T:45:LYS:HE2  | 19:T:49:LYS:HD2   | 1.98                     | 0.45              |
| 20:U:52:LEU:HD23 | 20:U:52:LEU:H     | 1.80                     | 0.45              |
| 31:f:121:CYS:SG  | 31:f:130:VAL:HG23 | 2.56                     | 0.45              |
| 37:z:581:A:H2'   | 37:z:582:U:C6     | 2.51                     | 0.45              |
| 1:2:552:U:C4'    | 11:L:132:GLN:HE22 | 2.29                     | 0.45              |
| 1:2:1618:A:C8    | 20:U:132:ARG:HG2  | 2.52                     | 0.45              |
| 5:F:218:LEU:HD21 | 32:g:172:LYS:HE2  | 1.99                     | 0.45              |
| 17:R:7:LYS:O     | 17:R:9:LYS:NZ     | 2.38                     | 0.45              |
| 18:S:29:ASN:N    | 18:S:67:ASP:OD1   | 2.47                     | 0.45              |
| 18:S:80:GLN:O    | 18:S:84:ILE:HG12  | 2.16                     | 0.45              |
| 32:g:45:LEU:HD22 | 32:g:52:TYR:CE2   | 2.51                     | 0.45              |
| 35:l:7:LYS:O     | 35:l:11:ARG:HG3   | 2.17                     | 0.45              |
| 1:2:565:A:H2'    | 1:2:566:A:O4'     | 2.17                     | 0.45              |
| 1:2:1054:A:H2'   | 1:2:1055:G:O4'    | 2.16                     | 0.45              |
| 1:2:1244:U:C2    | 36:y:33:C:H5'     | 2.51                     | 0.45              |
| 1:2:1300:U:H2'   | 1:2:1301:C:C6     | 2.52                     | 0.45              |
| 1:2:1309:A:O2'   | 14:O:91:LEU:HB2   | 2.17                     | 0.45              |
| 1:2:1384:A:H5''  | 19:T:45:LYS:NZ    | 2.32                     | 0.45              |
| 4:E:185:ARG:O    | 11:L:98:LEU:HD11  | 2.17                     | 0.45              |
| 5:F:67:ARG:NE    | 12:M:93:THR:HA    | 2.31                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:G:10:LYS:HA    | 6:G:27:PHE:HA     | 1.98                     | 0.45              |
| 6:G:137:PRO:HG2  | 6:G:150:PRO:HD2   | 1.99                     | 0.45              |
| 8:I:38:ALA:N     | 8:I:48:TYR:O      | 2.50                     | 0.45              |
| 9:J:73:GLN:HB3   | 9:J:135:PHE:CZ    | 2.51                     | 0.45              |
| 10:K:69:SER:HB3  | 13:N:20:LYS:HZ3   | 1.81                     | 0.45              |
| 11:L:42:GLU:OE1  | 11:L:42:GLU:N     | 2.42                     | 0.45              |
| 13:N:27:GLU:HA   | 13:N:28:THR:HA    | 1.61                     | 0.45              |
| 20:U:51:ASP:OD1  | 20:U:52:LEU:N     | 2.50                     | 0.45              |
| 22:W:32:LEU:HD21 | 22:W:85:HIS:HB2   | 1.97                     | 0.45              |
| 22:W:61:LEU:O    | 22:W:81:GLN:HA    | 2.16                     | 0.45              |
| 32:g:153:CYS:HB3 | 32:g:198:VAL:HG22 | 1.99                     | 0.45              |
| 36:y:48:G:H2'    | 36:y:49:A:C8      | 2.52                     | 0.45              |
| 36:y:64:C:H2'    | 36:y:65:C:C6      | 2.51                     | 0.45              |
| 37:z:596:A:H2'   | 37:z:597:A:H8     | 1.82                     | 0.45              |
| 1:2:386:U:H4'    | 10:K:14:THR:HG22  | 1.98                     | 0.45              |
| 1:2:800:U:H2'    | 1:2:801:U:C6      | 2.51                     | 0.45              |
| 1:2:834:G:N3     | 1:2:836:C:N4      | 2.65                     | 0.45              |
| 1:2:899:A:H2'    | 1:2:900:A:C8      | 2.52                     | 0.45              |
| 1:2:1089:A:H2'   | 1:2:1090:C:C6     | 2.52                     | 0.45              |
| 1:2:1839:A:H2'   | 1:2:1840:G:C8     | 2.52                     | 0.45              |
| 2:C:130:ASP:O    | 2:C:134:LEU:HD23  | 2.17                     | 0.45              |
| 3:D:23:ASP:O     | 3:D:26:SER:OG     | 2.29                     | 0.45              |
| 10:K:22:HIS:HB2  | 10:K:25:ARG:NH1   | 2.32                     | 0.45              |
| 13:N:38:LYS:NZ   | 13:N:39:ASN:OD1   | 2.28                     | 0.45              |
| 20:U:24:ARG:HD2  | 20:U:28:PHE:HB2   | 1.98                     | 0.45              |
| 20:U:104:ASP:N   | 20:U:104:ASP:OD1  | 2.47                     | 0.45              |
| 31:f:110:GLU:O   | 31:f:113:LYS:N    | 2.50                     | 0.45              |
| 31:f:146:LEU:HG  | 31:f:147:THR:HG23 | 1.99                     | 0.45              |
| 1:2:77:A:C6      | 8:I:181:THR:HG21  | 2.52                     | 0.45              |
| 1:2:575:C:OP2    | 11:L:172:ARG:NH1  | 2.49                     | 0.45              |
| 1:2:820:C:N3     | 11:L:144:ILE:HG13 | 2.31                     | 0.45              |
| 1:2:1570:G:H2'   | 1:2:1571:G:H8     | 1.81                     | 0.45              |
| 1:2:1675:G:H4'   | 29:d:20:ARG:HD3   | 1.98                     | 0.45              |
| 3:D:214:LYS:HB3  | 3:D:216:LYS:HZ3   | 1.82                     | 0.45              |
| 6:G:136:ILE:HG23 | 6:G:149:TYR:CD1   | 2.52                     | 0.45              |
| 7:H:36:GLN:C     | 7:H:38:TYR:H      | 2.25                     | 0.45              |
| 10:K:45:THR:HG22 | 10:K:53:LYS:HD2   | 1.99                     | 0.45              |
| 11:L:22:LYS:HA   | 11:L:22:LYS:HD2   | 1.84                     | 0.45              |
| 12:M:15:LEU:HD13 | 12:M:21:MET:HB2   | 1.99                     | 0.45              |
| 14:O:50:CYS:O    | 14:O:77:ILE:N     | 2.49                     | 0.45              |
| 1:2:65:C:C6      | 8:I:174:PRO:HB3   | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:895:U:H2'     | 1:2:896:C:O4'     | 2.17                     | 0.45              |
| 1:2:988:A:N7      | 27:b:15:ARG:NH1   | 2.65                     | 0.45              |
| 1:2:1431:C:H2'    | 1:2:1432:C:C4     | 2.52                     | 0.45              |
| 2:C:182:VAL:O     | 2:C:186:ARG:HD3   | 2.17                     | 0.45              |
| 5:F:50:ILE:O      | 5:F:89:GLU:HG3    | 2.16                     | 0.45              |
| 7:H:47:LYS:HZ2    | 18:S:115:TYR:HE1  | 1.64                     | 0.45              |
| 9:J:143:ARG:NH1   | 24:Y:53:ILE:HA    | 2.32                     | 0.45              |
| 14:O:85:LEU:HD23  | 14:O:107:SER:H    | 1.81                     | 0.45              |
| 17:R:14:LYS:HE2   | 37:z:563:C:H2'    | 1.99                     | 0.45              |
| 19:T:54:VAL:HA    | 19:T:57:LEU:HD13  | 1.99                     | 0.45              |
| 19:T:121:GLN:NE2  | 19:T:122:PRO:O    | 2.50                     | 0.45              |
| 20:U:64:VAL:O     | 20:U:68:ILE:HG13  | 2.17                     | 0.45              |
| 23:X:67:ASP:HA    | 23:X:70:LEU:HG    | 1.98                     | 0.45              |
| 28:c:13:GLU:O     | 28:c:17:ARG:HB2   | 2.17                     | 0.45              |
| 31:f:106:TYR:CG   | 31:f:114:ILE:HD12 | 2.52                     | 0.45              |
| 32:g:152:SER:H    | 32:g:169:GLY:HA2  | 1.82                     | 0.45              |
| 1:2:371:C:OP2     | 10:K:31:ARG:NH2   | 2.50                     | 0.45              |
| 1:2:1119:C:O3'    | 3:D:149:GLN:HG3   | 2.17                     | 0.45              |
| 6:G:86:PHE:HE1    | 6:G:102:ILE:HA    | 1.81                     | 0.45              |
| 13:N:4:ILE:HD11   | 13:N:54:THR:HG23  | 1.98                     | 0.45              |
| 21:V:27:LYS:HB3   | 21:V:110:LEU:HD21 | 1.98                     | 0.45              |
| 22:W:20:ILE:HG13  | 22:W:115:THR:O    | 2.17                     | 0.45              |
| 37:z:525:A:H3'    | 37:z:526:G:H21    | 1.82                     | 0.45              |
| 37:z:564:G:H22    | 37:z:574:C:H1'    | 1.82                     | 0.45              |
| 1:2:72:C:H4'      | 1:2:73:C:H6       | 1.81                     | 0.44              |
| 1:2:580:A:H4'     | 34:i:98:LYS:HE2   | 1.98                     | 0.44              |
| 1:2:831:C:O2'     | 1:2:832:G:N2      | 2.50                     | 0.44              |
| 1:2:1506:G:H2'    | 1:2:1506:G:N3     | 2.32                     | 0.44              |
| 1:2:1736:U:OP1    | 10:K:42:ARG:HD3   | 2.17                     | 0.44              |
| 1:2:1803:A:H2'    | 1:2:1804:U:H6     | 1.82                     | 0.44              |
| 4:E:207:CYS:SG    | 4:E:208:TYR:N     | 2.90                     | 0.44              |
| 7:H:67:PRO:O      | 7:H:70:GLU:HB3    | 2.17                     | 0.44              |
| 11:L:21:GLU:OE1   | 11:L:24:ARG:N     | 2.38                     | 0.44              |
| 12:M:27:VAL:HG23  | 12:M:28:HIS:CE1   | 2.52                     | 0.44              |
| 17:R:25:LEU:HB3   | 17:R:87:PRO:HG3   | 1.99                     | 0.44              |
| 20:U:108:ARG:HA   | 20:U:111:LEU:HD13 | 1.99                     | 0.44              |
| 20:U:109:GLU:O    | 20:U:113:ARG:N    | 2.40                     | 0.44              |
| 31:f:146:LEU:HD23 | 31:f:146:LEU:H    | 1.82                     | 0.44              |
| 37:z:592:C:H2'    | 37:z:593:U:H6     | 1.81                     | 0.44              |
| 1:2:223:A:C5      | 1:2:277:U:H5'     | 2.52                     | 0.44              |
| 1:2:343:C:H4'     | 13:N:90:ARG:HH12  | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:384:G:H4'    | 13:N:82:MET:HE1  | 1.98                     | 0.44              |
| 1:2:1195:A:H5''  | 27:b:2:THR:HG22  | 1.99                     | 0.44              |
| 1:2:1355:U:H2'   | 1:2:1356:U:C6    | 2.51                     | 0.44              |
| 1:2:1494:A:OP2   | 5:F:27:ARG:NH2   | 2.50                     | 0.44              |
| 1:2:1674:A:OP1   | 7:H:60:ARG:NH1   | 2.50                     | 0.44              |
| 1:2:1789:G:H2'   | 1:2:1790:G:C8    | 2.51                     | 0.44              |
| 2:C:73:ASP:OD1   | 2:C:73:ASP:N     | 2.50                     | 0.44              |
| 4:E:79:ILE:HG21  | 4:E:144:LYS:O    | 2.17                     | 0.44              |
| 6:G:62:LYS:HA    | 6:G:65:CYS:SG    | 2.58                     | 0.44              |
| 8:I:44:GLU:HG3   | 8:I:119:LYS:HB2  | 1.99                     | 0.44              |
| 16:Q:141:ARG:HG2 | 27:b:22:ARG:NH2  | 2.33                     | 0.44              |
| 17:R:59:ARG:O    | 17:R:63:ALA:N    | 2.44                     | 0.44              |
| 22:W:56:MET:HE3  | 22:W:86:LYS:HE2  | 2.00                     | 0.44              |
| 25:Z:57:VAL:HG23 | 25:Z:67:ARG:HB2  | 1.98                     | 0.44              |
| 29:d:16:LYS:O    | 29:d:31:ARG:N    | 2.48                     | 0.44              |
| 37:z:521:U:H2'   | 37:z:522:U:H6    | 1.81                     | 0.44              |
| 1:2:12:U:H2'     | 1:2:13:C:H6      | 1.82                     | 0.44              |
| 1:2:189:G:H1'    | 1:2:206:A:H61    | 1.82                     | 0.44              |
| 1:2:497:G:OP1    | 26:a:108:LYS:NZ  | 2.41                     | 0.44              |
| 1:2:573:A:H2'    | 1:2:573:A:N3     | 2.33                     | 0.44              |
| 1:2:1088:G:OP1   | 15:P:2:GLY:N     | 2.50                     | 0.44              |
| 1:2:1117:G:C6    | 1:2:1118:A:C5    | 3.05                     | 0.44              |
| 1:2:1176:C:H2'   | 1:2:1177:A:O4'   | 2.18                     | 0.44              |
| 1:2:1326:G:N2    | 1:2:1331:G:O6    | 2.50                     | 0.44              |
| 1:2:1414:C:H4'   | 1:2:1415:C:H5'   | 2.00                     | 0.44              |
| 1:2:1442:A:H4'   | 22:W:87:ARG:HH22 | 1.83                     | 0.44              |
| 1:2:1603:U:H2'   | 1:2:1604:C:O4'   | 2.17                     | 0.44              |
| 1:2:1697:G:O6    | 1:2:1830:G:N2    | 2.50                     | 0.44              |
| 9:J:87:PHE:HB3   | 9:J:90:LYS:HD2   | 1.98                     | 0.44              |
| 11:L:54:ARG:HH12 | 11:L:98:LEU:HA   | 1.82                     | 0.44              |
| 12:M:48:ALA:O    | 12:M:51:SER:OG   | 2.34                     | 0.44              |
| 18:S:10:VAL:HG11 | 18:S:98:LYS:HE2  | 1.98                     | 0.44              |
| 18:S:82:TYR:O    | 18:S:86:GLN:HG3  | 2.16                     | 0.44              |
| 19:T:73:LEU:O    | 19:T:76:GLU:HG2  | 2.18                     | 0.44              |
| 21:V:87:VAL:HG13 | 21:V:88:MET:HE2  | 1.98                     | 0.44              |
| 24:Y:15:ASN:ND2  | 24:Y:72:CYS:SG   | 2.91                     | 0.44              |
| 24:Y:87:GLU:OE2  | 24:Y:117:ARG:NH2 | 2.50                     | 0.44              |
| 26:a:24:VAL:HB   | 26:a:72:PHE:CD1  | 2.52                     | 0.44              |
| 36:y:46:U:H4'    | 36:y:47:C:H5     | 1.82                     | 0.44              |
| 37:z:596:A:H2'   | 37:z:597:A:C8    | 2.53                     | 0.44              |
| 1:2:479:A:H2'    | 1:2:480:C:H6     | 1.83                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:799:C:H2'    | 1:2:800:U:H6     | 1.82                     | 0.44              |
| 1:2:1063:C:H2'   | 1:2:1064:G:C8    | 2.53                     | 0.44              |
| 1:2:1123:C:C4'   | 28:c:17:ARG:HH12 | 2.30                     | 0.44              |
| 1:2:1383:G:C2    | 1:2:1384:A:H1'   | 2.52                     | 0.44              |
| 1:2:1513:C:H5''  | 1:2:1514:U:H5''  | 1.99                     | 0.44              |
| 1:2:1558:G:C6    | 1:2:1559:C:C4    | 3.05                     | 0.44              |
| 1:2:1667:U:H2'   | 1:2:1668:U:H6    | 1.83                     | 0.44              |
| 3:D:112:SER:HA   | 27:b:68:TYR:HE2  | 1.83                     | 0.44              |
| 6:G:49:ARG:HD3   | 6:G:61:VAL:HG21  | 1.98                     | 0.44              |
| 6:G:247:THR:HG23 | 6:G:250:GLU:H    | 1.80                     | 0.44              |
| 8:I:77:LEU:N     | 8:I:93:LYS:O     | 2.41                     | 0.44              |
| 12:M:90:VAL:HG13 | 12:M:90:VAL:O    | 2.17                     | 0.44              |
| 15:P:142:GLU:OE1 | 15:P:144:SER:OG  | 2.29                     | 0.44              |
| 19:T:17:ILE:HD11 | 19:T:21:TYR:CD1  | 2.51                     | 0.44              |
| 22:W:78:ASP:OD1  | 22:W:78:ASP:N    | 2.50                     | 0.44              |
| 31:f:135:HIS:CD2 | 31:f:140:TYR:HB3 | 2.53                     | 0.44              |
| 36:y:21:G:H2'    | 36:y:22:C:H6     | 1.80                     | 0.44              |
| 1:2:145:G:H2'    | 1:2:146:G:H8     | 1.82                     | 0.44              |
| 1:2:198:U:H3'    | 1:2:199:G:H8     | 1.82                     | 0.44              |
| 1:2:639:U:OP2    | 25:Z:106:GLY:HA2 | 2.16                     | 0.44              |
| 1:2:957:G:N3     | 37:z:831:A:C6    | 2.86                     | 0.44              |
| 1:2:1028:C:H5''  | 15:P:109:LYS:HZ2 | 1.82                     | 0.44              |
| 1:2:1135:C:H3'   | 1:2:1136:G:C8    | 2.53                     | 0.44              |
| 1:2:1144:A:H4'   | 1:2:1145:A:O4'   | 2.17                     | 0.44              |
| 1:2:1294:G:N3    | 17:R:79:HIS:CE1  | 2.85                     | 0.44              |
| 1:2:1407:G:H3'   | 1:2:1408:C:H5''  | 2.00                     | 0.44              |
| 1:2:1517:A:O2'   | 20:U:143:GLY:O   | 2.27                     | 0.44              |
| 1:2:1586:C:H5''  | 7:H:88:MET:HE3   | 1.99                     | 0.44              |
| 2:C:56:GLU:OE1   | 23:X:79:VAL:HA   | 2.17                     | 0.44              |
| 4:E:153:GLY:HA3  | 4:E:166:ARG:HA   | 1.99                     | 0.44              |
| 6:G:29:PRO:HG3   | 6:G:45:ILE:HD11  | 2.00                     | 0.44              |
| 10:K:125:LYS:HG3 | 10:K:128:LYS:H   | 1.83                     | 0.44              |
| 12:M:26:ASP:CB   | 12:M:29:MET:HB2  | 2.47                     | 0.44              |
| 20:U:6:PRO:O     | 33:h:49:LEU:HD12 | 2.17                     | 0.44              |
| 22:W:61:LEU:H    | 22:W:83:ARG:HH21 | 1.65                     | 0.44              |
| 22:W:82:MET:HA   | 22:W:82:MET:HE2  | 1.99                     | 0.44              |
| 32:g:131:LEU:HB3 | 32:g:139:LYS:HB3 | 1.99                     | 0.44              |
| 37:z:540:C:H2'   | 37:z:541:C:H6    | 1.83                     | 0.44              |
| 1:2:185:C:H2'    | 1:2:186:G:H8     | 1.83                     | 0.44              |
| 1:2:215:U:H2'    | 1:2:216:U:C6     | 2.52                     | 0.44              |
| 1:2:864:G:O2'    | 9:J:112:ASN:O    | 2.30                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1103:G:H2'    | 1:2:1104:G:H8     | 1.83                     | 0.44              |
| 1:2:1286:G:N2     | 1:2:1306:U:H1'    | 2.33                     | 0.44              |
| 1:2:1300:U:H4'    | 31:f:92:LYS:HD3   | 2.00                     | 0.44              |
| 1:2:1643:G:O2'    | 18:S:127:CYS:SG   | 2.59                     | 0.44              |
| 4:E:72:PRO:HG3    | 23:X:29:HIS:CG    | 2.52                     | 0.44              |
| 7:H:113:VAL:HA    | 7:H:116:ILE:HB    | 1.99                     | 0.44              |
| 7:H:118:ASN:ND2   | 7:H:181:ALA:O     | 2.50                     | 0.44              |
| 8:I:111:LEU:HD23  | 8:I:111:LEU:H     | 1.82                     | 0.44              |
| 15:P:19:ARG:HD3   | 15:P:20:ARG:H     | 1.82                     | 0.44              |
| 16:Q:95:ILE:HB    | 16:Q:129:ILE:HG22 | 2.00                     | 0.44              |
| 19:T:92:ASP:OD1   | 19:T:92:ASP:N     | 2.49                     | 0.44              |
| 24:Y:102:ILE:HG12 | 24:Y:113:HIS:CD2  | 2.49                     | 0.44              |
| 26:a:12:PHE:CZ    | 26:a:21:LYS:HD2   | 2.51                     | 0.44              |
| 27:b:41:ILE:HG22  | 27:b:68:TYR:CE1   | 2.53                     | 0.44              |
| 36:y:9:G:N7       | 36:y:19:A:O2'     | 2.51                     | 0.44              |
| 36:y:48:G:N2      | 37:z:550:A:HO2'   | 2.14                     | 0.44              |
| 1:2:83:A:C5       | 1:2:84:A:C8       | 3.04                     | 0.44              |
| 1:2:397:G:OP1     | 1:2:397:G:N2      | 2.38                     | 0.44              |
| 1:2:485:U:H2'     | 1:2:486:C:O4'     | 2.18                     | 0.44              |
| 1:2:746:C:H2'     | 1:2:747:G:N9      | 2.33                     | 0.44              |
| 1:2:1103:G:OP2    | 28:c:70:LYS:NZ    | 2.50                     | 0.44              |
| 1:2:1123:C:H2'    | 1:2:1124:C:H6     | 1.82                     | 0.44              |
| 1:2:1154:G:C6     | 1:2:1155:G:C6     | 3.05                     | 0.44              |
| 1:2:1283:A:N6     | 1:2:1284:U:O2     | 2.51                     | 0.44              |
| 1:2:1412:C:H2'    | 1:2:1413:C:C6     | 2.53                     | 0.44              |
| 1:2:1447:G:O2'    | 1:2:1470:A:N6     | 2.51                     | 0.44              |
| 1:2:1535:G:H2'    | 1:2:1536:G:C8     | 2.53                     | 0.44              |
| 1:2:1614:A:OP2    | 17:R:47:ARG:NH2   | 2.39                     | 0.44              |
| 1:2:1626:U:H2'    | 1:2:1627:G:O4'    | 2.18                     | 0.44              |
| 3:D:84:PHE:CE1    | 3:D:103:MET:HB3   | 2.52                     | 0.44              |
| 6:G:195:ILE:HG23  | 6:G:196:THR:N     | 2.32                     | 0.44              |
| 11:L:93:LYS:HD2   | 11:L:93:LYS:HA    | 1.84                     | 0.44              |
| 17:R:79:HIS:CD2   | 17:R:97:TYR:CD2   | 3.05                     | 0.44              |
| 18:S:45:ARG:NH1   | 21:V:10:ASN:HD21  | 2.16                     | 0.44              |
| 20:U:109:GLU:N    | 20:U:109:GLU:OE1  | 2.50                     | 0.44              |
| 25:Z:102:VAL:HA   | 25:Z:122:VAL:HA   | 2.00                     | 0.44              |
| 26:a:38:THR:O     | 26:a:41:GLN:HG2   | 2.17                     | 0.44              |
| 36:y:19:A:H1'     | 36:y:58:A:C8      | 2.52                     | 0.44              |
| 1:2:285:U:O4      | 13:N:14:PRO:HG2   | 2.18                     | 0.44              |
| 1:2:469:C:C2      | 1:2:470:G:C8      | 3.05                     | 0.44              |
| 1:2:560:C:H2'     | 1:2:561:U:C6      | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:750:G:H2'    | 1:2:751:C:C6     | 2.53                     | 0.44              |
| 1:2:829:C:H1'    | 6:G:262:SER:HB2  | 2.00                     | 0.44              |
| 1:2:1465:A:H2'   | 1:2:1466:C:H6    | 1.82                     | 0.44              |
| 2:C:11:LYS:H     | 2:C:55:TRP:HH2   | 1.63                     | 0.44              |
| 2:C:33:GLN:C     | 2:C:34:MET:HE2   | 2.43                     | 0.44              |
| 2:C:120:ARG:NE   | 4:E:252:GLN:OE1  | 2.51                     | 0.44              |
| 4:E:120:GLY:O    | 4:E:150:VAL:HG22 | 2.18                     | 0.44              |
| 6:G:180:LEU:HB3  | 6:G:228:ILE:HG22 | 2.00                     | 0.44              |
| 7:H:46:ALA:O     | 7:H:47:LYS:NZ    | 2.49                     | 0.44              |
| 9:J:27:LEU:O     | 9:J:31:GLU:HG2   | 2.18                     | 0.44              |
| 22:W:61:LEU:HD12 | 22:W:62:ARG:H    | 1.82                     | 0.44              |
| 32:g:280:LYS:HD2 | 32:g:280:LYS:HA  | 1.83                     | 0.44              |
| 36:y:67:C:H2'    | 36:y:68:U:H6     | 1.83                     | 0.44              |
| 1:2:471:C:H2'    | 1:2:472:G:C8     | 2.53                     | 0.44              |
| 1:2:679:U:H2'    | 1:2:680:G:C8     | 2.53                     | 0.44              |
| 1:2:939:U:H2'    | 1:2:940:A:H8     | 1.83                     | 0.44              |
| 1:2:1051:A:C5    | 1:2:1052:U:C4    | 3.06                     | 0.44              |
| 1:2:1447:G:C2'   | 1:2:1470:A:H61   | 2.31                     | 0.44              |
| 1:2:1453:U:H2'   | 1:2:1454:G:H8    | 1.83                     | 0.44              |
| 1:2:1774:G:O6    | 1:2:1775:A:N6    | 2.51                     | 0.44              |
| 1:2:1858:U:O4    | 27:b:34:LYS:NZ   | 2.44                     | 0.44              |
| 2:C:9:GLN:HG3    | 2:C:10:MET:H     | 1.82                     | 0.44              |
| 3:D:107:ARG:HA   | 3:D:110:MET:HG3  | 2.00                     | 0.44              |
| 5:F:28:GLU:HG3   | 5:F:29:LEU:HG    | 1.99                     | 0.44              |
| 12:M:7:ASN:O     | 12:M:11:ILE:HG12 | 2.18                     | 0.44              |
| 37:z:581:A:H2'   | 37:z:582:U:H6    | 1.83                     | 0.44              |
| 1:2:115:U:H2'    | 1:2:116:U:C6     | 2.53                     | 0.43              |
| 1:2:170:A:OP1    | 8:I:137:ARG:HG3  | 2.18                     | 0.43              |
| 1:2:214:A:H61    | 1:2:295:C:N4     | 2.16                     | 0.43              |
| 1:2:811:U:N3     | 1:2:812:A:N7     | 2.66                     | 0.43              |
| 1:2:843:A:H2'    | 1:2:844:U:O4'    | 2.18                     | 0.43              |
| 1:2:1102:C:OP1   | 28:c:70:LYS:NZ   | 2.37                     | 0.43              |
| 1:2:1289:A:H1'   | 31:f:138:ARG:HD3 | 2.00                     | 0.43              |
| 1:2:1369:C:OP1   | 19:T:7:LYS:HG2   | 2.18                     | 0.43              |
| 1:2:1487:G:H2'   | 1:2:1488:U:C6    | 2.53                     | 0.43              |
| 2:C:89:LYS:HZ3   | 2:C:202:TYR:HD1  | 1.65                     | 0.43              |
| 2:C:123:VAL:HA   | 2:C:145:ILE:HG23 | 2.00                     | 0.43              |
| 3:D:147:ASN:OD1  | 3:D:148:ASN:N    | 2.51                     | 0.43              |
| 6:G:35:PRO:HG2   | 6:G:36:HIS:ND1   | 2.33                     | 0.43              |
| 6:G:125:LYS:HB2  | 6:G:226:PHE:CD1  | 2.52                     | 0.43              |
| 7:H:18:LYS:HZ3   | 7:H:48:TYR:HE2   | 1.66                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:H:78:MET:HG2    | 7:H:79:HIS:CG     | 2.53                     | 0.43              |
| 8:I:63:MET:HE1    | 8:I:98:ARG:HD2    | 2.00                     | 0.43              |
| 12:M:32:HIS:HB2   | 12:M:40:VAL:HB    | 2.00                     | 0.43              |
| 14:O:99:LYS:HZ2   | 14:O:102:LYS:HG3  | 1.82                     | 0.43              |
| 28:c:21:LYS:NZ    | 28:c:26:GLN:OE1   | 2.50                     | 0.43              |
| 1:2:11:A:N1       | 1:2:1196:A:H2     | 2.16                     | 0.43              |
| 1:2:673:G:N1      | 1:2:1018:U:OP2    | 2.46                     | 0.43              |
| 1:2:924:G:H2'     | 1:2:925:G:C8      | 2.53                     | 0.43              |
| 1:2:1206:G:H2'    | 1:2:1207:G:C8     | 2.53                     | 0.43              |
| 1:2:1255:A:H1'    | 1:2:1260:C:H42    | 1.82                     | 0.43              |
| 1:2:1261:A:H2'    | 1:2:1261:A:N3     | 2.33                     | 0.43              |
| 4:E:78:ILE:H      | 4:E:78:ILE:HD12   | 1.82                     | 0.43              |
| 10:K:114:GLU:CD   | 10:K:123:ARG:HH22 | 2.27                     | 0.43              |
| 11:L:147:PHE:HD2  | 11:L:149:VAL:HG22 | 1.82                     | 0.43              |
| 12:M:1:MET:N      | 12:M:2:LEU:HB3    | 2.31                     | 0.43              |
| 14:O:58:GLU:OE2   | 31:f:104:LYS:NZ   | 2.51                     | 0.43              |
| 22:W:24:LEU:N     | 22:W:87:ARG:O     | 2.39                     | 0.43              |
| 26:a:35:VAL:HG23  | 26:a:40:ILE:HD11  | 2.00                     | 0.43              |
| 37:z:582:U:N3     | 37:z:585:G:OP2    | 2.37                     | 0.43              |
| 1:2:94:G:HO2'     | 1:2:498:A:HO2'    | 1.60                     | 0.43              |
| 1:2:528:U:H2'     | 1:2:529:C:C6      | 2.53                     | 0.43              |
| 1:2:799:C:H2'     | 1:2:800:U:C6      | 2.54                     | 0.43              |
| 1:2:1154:G:N1     | 1:2:1155:G:C6     | 2.86                     | 0.43              |
| 1:2:1194:G:H2'    | 1:2:1195:A:C8     | 2.53                     | 0.43              |
| 1:2:1386:U:H2'    | 1:2:1387:C:H6     | 1.84                     | 0.43              |
| 1:2:1450:A:OP1    | 19:T:49:LYS:NZ    | 2.50                     | 0.43              |
| 1:2:1474:U:H2'    | 1:2:1475:G:H8     | 1.77                     | 0.43              |
| 1:2:1721:G:H2'    | 1:2:1722:G:H8     | 1.84                     | 0.43              |
| 2:C:80:ARG:NE     | 2:C:81:ASN:OD1    | 2.51                     | 0.43              |
| 3:D:177:GLN:NE2   | 3:D:178:THR:HG23  | 2.32                     | 0.43              |
| 4:E:168:LYS:HD2   | 4:E:179:ARG:NE    | 2.33                     | 0.43              |
| 6:G:70:ILE:C      | 6:G:71:LYS:HD3    | 2.44                     | 0.43              |
| 7:H:56:TYR:OH     | 7:H:66:CYS:HB2    | 2.19                     | 0.43              |
| 11:L:86:VAL:HG23  | 11:L:87:LEU:HD12  | 2.01                     | 0.43              |
| 16:Q:31:CYS:SG    | 16:Q:93:LEU:HD12  | 2.58                     | 0.43              |
| 20:U:40:TYR:HA    | 20:U:83:PHE:CE2   | 2.53                     | 0.43              |
| 24:Y:32:LYS:HG3   | 24:Y:36:ARG:HH21  | 1.82                     | 0.43              |
| 32:g:31:ILE:HG23  | 32:g:43:TRP:CD1   | 2.53                     | 0.43              |
| 32:g:33:SER:CB    | 32:g:43:TRP:HE1   | 2.31                     | 0.43              |
| 32:g:197:THR:HG21 | 32:g:238:ALA:HA   | 1.99                     | 0.43              |
| 32:g:206:LEU:HD12 | 32:g:219:TRP:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:221:A:H2'    | 1:2:222:G:O4'    | 2.18                     | 0.43              |
| 1:2:290:A:H2'    | 1:2:291:U:C6     | 2.53                     | 0.43              |
| 1:2:649:G:O4'    | 1:2:652:G:N2     | 2.50                     | 0.43              |
| 1:2:868:A:H1'    | 1:2:869:G:H5'    | 2.00                     | 0.43              |
| 1:2:1155:G:OP2   | 25:Z:5:ARG:NH1   | 2.50                     | 0.43              |
| 2:C:90:PHE:CD2   | 2:C:175:TRP:HZ3  | 2.36                     | 0.43              |
| 5:F:22:ASN:HD21  | 30:e:46:TYR:HE1  | 1.66                     | 0.43              |
| 5:F:141:LYS:O    | 5:F:142:LEU:HD23 | 2.19                     | 0.43              |
| 6:G:15:PRO:HG3   | 6:G:39:ARG:CZ    | 2.48                     | 0.43              |
| 6:G:100:ARG:O    | 6:G:112:HIS:HB2  | 2.18                     | 0.43              |
| 6:G:128:LYS:HE2  | 6:G:140:VAL:HG11 | 1.99                     | 0.43              |
| 9:J:80:VAL:HG13  | 9:J:92:VAL:HG13  | 2.00                     | 0.43              |
| 20:U:118:ARG:NE  | 37:z:569:A:OP1   | 2.39                     | 0.43              |
| 22:W:28:ASN:HB2  | 22:W:31:SER:HB2  | 1.99                     | 0.43              |
| 25:Z:103:ALA:O   | 25:Z:121:LYS:N   | 2.50                     | 0.43              |
| 29:d:31:ARG:NH1  | 29:d:43:ILE:HG12 | 2.33                     | 0.43              |
| 31:f:119:ARG:CZ  | 31:f:132:MET:HE2 | 2.48                     | 0.43              |
| 1:2:163:U:O3'    | 8:I:83:CYS:HA    | 2.18                     | 0.43              |
| 1:2:186:G:H2'    | 1:2:187:C:C6     | 2.53                     | 0.43              |
| 1:2:520:U:H3     | 1:2:544:A:H62    | 1.65                     | 0.43              |
| 1:2:1123:C:H4'   | 28:c:17:ARG:NH1  | 2.31                     | 0.43              |
| 1:2:1167:G:N2    | 1:2:1184:A:OP2   | 2.52                     | 0.43              |
| 1:2:1637:U:H2'   | 1:2:1638:U:C6    | 2.54                     | 0.43              |
| 2:C:58:LEU:HD12  | 2:C:178:LEU:HD13 | 2.01                     | 0.43              |
| 2:C:155:ARG:HG2  | 2:C:156:TYR:HD1  | 1.83                     | 0.43              |
| 15:P:126:ALA:HB1 | 15:P:139:TRP:HZ3 | 1.83                     | 0.43              |
| 20:U:23:ARG:HH12 | 33:h:47:LEU:HA   | 1.83                     | 0.43              |
| 22:W:27:ARG:NH2  | 30:e:51:GLY:O    | 2.51                     | 0.43              |
| 22:W:81:GLN:HB3  | 22:W:83:ARG:NH2  | 2.32                     | 0.43              |
| 26:a:44:LEU:O    | 26:a:47:MET:HB3  | 2.19                     | 0.43              |
| 28:c:35:VAL:HB   | 28:c:63:LEU:HD21 | 1.99                     | 0.43              |
| 37:z:580:U:H2'   | 37:z:581:A:C8    | 2.54                     | 0.43              |
| 1:2:1195:A:OP1   | 27:b:2:THR:N     | 2.51                     | 0.43              |
| 3:D:81:PHE:CD1   | 3:D:109:LYS:HE2  | 2.53                     | 0.43              |
| 7:H:51:HIS:ND1   | 18:S:82:TYR:OH   | 2.39                     | 0.43              |
| 8:I:201:LYS:HA   | 8:I:201:LYS:HD3  | 1.86                     | 0.43              |
| 9:J:75:ILE:HG23  | 9:J:76:GLN:N     | 2.32                     | 0.43              |
| 10:K:4:SER:HA    | 10:K:28:GLU:OE1  | 2.19                     | 0.43              |
| 10:K:48:VAL:HG12 | 10:K:52:ASN:O    | 2.18                     | 0.43              |
| 16:Q:28:PHE:HB2  | 16:Q:47:LEU:HD11 | 2.00                     | 0.43              |
| 1:2:282:G:H21    | 13:N:41:GLY:HA3  | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:296:U:H5''   | 1:2:297:C:C2     | 2.53                     | 0.43              |
| 1:2:479:A:H2'    | 1:2:480:C:C6     | 2.54                     | 0.43              |
| 1:2:602:U:C5     | 1:2:603:C:H5     | 2.37                     | 0.43              |
| 1:2:812:A:H2'    | 1:2:813:G:C8     | 2.53                     | 0.43              |
| 1:2:943:G:H2'    | 1:2:944:C:H6     | 1.84                     | 0.43              |
| 1:2:952:G:H2'    | 1:2:953:A:H8     | 1.83                     | 0.43              |
| 1:2:1282:G:O6    | 14:O:36:ARG:HB3  | 2.18                     | 0.43              |
| 1:2:1375:A:H2'   | 1:2:1376:C:H6    | 1.84                     | 0.43              |
| 1:2:1641:C:C4    | 1:2:1673:A:C8    | 3.06                     | 0.43              |
| 5:F:193:ASP:HB3  | 5:F:194:PRO:CD   | 2.46                     | 0.43              |
| 9:J:41:ARG:HA    | 9:J:41:ARG:HD2   | 1.74                     | 0.43              |
| 11:L:84:ILE:HG13 | 11:L:86:VAL:HG22 | 2.00                     | 0.43              |
| 17:R:86:LEU:HB3  | 17:R:87:PRO:HD2  | 2.01                     | 0.43              |
| 18:S:29:ASN:N    | 18:S:29:ASN:OD1  | 2.50                     | 0.43              |
| 21:V:139:ALA:HA  | 21:V:144:LYS:HB2 | 2.00                     | 0.43              |
| 25:Z:33:GLY:O    | 25:Z:36:LEU:HG   | 2.19                     | 0.43              |
| 32:g:101:PHE:CD1 | 32:g:136:GLY:HA2 | 2.54                     | 0.43              |
| 34:i:107:LYS:O   | 34:i:110:MET:HG3 | 2.19                     | 0.43              |
| 1:2:109:U:O2'    | 13:N:71:ARG:NH2  | 2.51                     | 0.43              |
| 1:2:554:A:H2'    | 1:2:555:G:O4'    | 2.19                     | 0.43              |
| 1:2:606:A:OP1    | 25:Z:66:ILE:HB   | 2.18                     | 0.43              |
| 1:2:744:C:H2'    | 1:2:745:U:C4     | 2.54                     | 0.43              |
| 1:2:900:A:H2'    | 1:2:901:C:C6     | 2.54                     | 0.43              |
| 1:2:942:U:C2     | 1:2:943:G:C8     | 3.07                     | 0.43              |
| 1:2:1028:C:H5''  | 15:P:109:LYS:NZ  | 2.33                     | 0.43              |
| 1:2:1220:G:H2'   | 1:2:1221:U:C6    | 2.54                     | 0.43              |
| 1:2:1614:A:P     | 17:R:47:ARG:HH21 | 2.42                     | 0.43              |
| 2:C:169:HIS:CE1  | 2:C:203:PHE:HB3  | 2.54                     | 0.43              |
| 4:E:195:PRO:HB3  | 4:E:221:PHE:HE1  | 1.83                     | 0.43              |
| 5:F:39:VAL:HG23  | 5:F:48:ILE:HG13  | 2.01                     | 0.43              |
| 5:F:164:VAL:O    | 5:F:168:VAL:HG22 | 2.18                     | 0.43              |
| 9:J:23:ILE:HG13  | 9:J:87:PHE:HE2   | 1.83                     | 0.43              |
| 9:J:66:VAL:HG13  | 9:J:69:LEU:HB2   | 2.01                     | 0.43              |
| 12:M:15:LEU:O    | 12:M:19:GLY:N    | 2.45                     | 0.43              |
| 15:P:142:GLU:H   | 15:P:145:THR:HG1 | 1.62                     | 0.43              |
| 19:T:25:GLY:O    | 19:T:58:MET:HG2  | 2.19                     | 0.43              |
| 27:b:23:CYS:HB3  | 27:b:28:CYS:H    | 1.84                     | 0.43              |
| 32:g:78:ALA:O    | 32:g:90:TRP:N    | 2.51                     | 0.43              |
| 32:g:119:GLN:HG2 | 32:g:139:LYS:NZ  | 2.34                     | 0.43              |
| 37:z:597:A:H2'   | 37:z:598:A:H8    | 1.83                     | 0.43              |
| 1:2:11:A:H5'     | 4:E:98:GLN:HE22  | 1.84                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:29:G:C6      | 1:2:636:G:C6     | 3.06                     | 0.43              |
| 1:2:51:U:H2'     | 1:2:52:G:H8      | 1.83                     | 0.43              |
| 1:2:331:C:H2'    | 1:2:332:C:H6     | 1.84                     | 0.43              |
| 1:2:951:A:H5''   | 16:Q:60:MET:HE2  | 2.00                     | 0.43              |
| 1:2:970:C:C2     | 1:2:971:G:C8     | 3.07                     | 0.43              |
| 1:2:1095:G:N2    | 1:2:1129:A:N1    | 2.56                     | 0.43              |
| 1:2:1194:G:H2'   | 1:2:1195:A:H8    | 1.84                     | 0.43              |
| 1:2:1252:G:O6    | 30:e:31:ILE:HD11 | 2.19                     | 0.43              |
| 1:2:1338:U:H3    | 1:2:1479:A:N6    | 2.17                     | 0.43              |
| 1:2:1462:G:H2'   | 1:2:1463:C:C6    | 2.54                     | 0.43              |
| 1:2:1497:C:H2'   | 1:2:1498:C:C6    | 2.54                     | 0.43              |
| 1:2:1589:A:H62   | 33:h:104:ARG:HD2 | 1.83                     | 0.43              |
| 5:F:23:GLU:HB2   | 30:e:46:TYR:OH   | 2.18                     | 0.43              |
| 6:G:160:ILE:HD12 | 6:G:169:ILE:HG21 | 2.00                     | 0.43              |
| 6:G:191:ARG:CZ   | 6:G:245:ARG:HE   | 2.32                     | 0.43              |
| 13:N:71:ARG:H    | 13:N:130:GLU:CD  | 2.26                     | 0.43              |
| 20:U:8:LYS:HD2   | 33:h:50:PHE:O    | 2.18                     | 0.43              |
| 22:W:61:LEU:HD23 | 22:W:82:MET:HG2  | 2.00                     | 0.43              |
| 23:X:39:VAL:HG23 | 23:X:41:LYS:H    | 1.84                     | 0.43              |
| 24:Y:15:ASN:ND2  | 24:Y:72:CYS:O    | 2.47                     | 0.43              |
| 1:2:2:A:C5       | 1:2:408:A:H1'    | 2.54                     | 0.43              |
| 1:2:332:C:H2'    | 1:2:333:A:H8     | 1.84                     | 0.43              |
| 1:2:411:G:O3'    | 13:N:98:LYS:NZ   | 2.52                     | 0.43              |
| 1:2:532:U:H2'    | 1:2:533:C:O4'    | 2.18                     | 0.43              |
| 1:2:818:U:H2'    | 1:2:820:C:OP2    | 2.19                     | 0.43              |
| 1:2:824:G:H4'    | 6:G:23:LEU:HD11  | 2.01                     | 0.43              |
| 1:2:924:G:C6     | 1:2:1010:G:C6    | 3.07                     | 0.43              |
| 1:2:1016:A:N7    | 15:P:70:LYS:NZ   | 2.67                     | 0.43              |
| 1:2:1195:A:H2'   | 1:2:1196:A:C8    | 2.54                     | 0.43              |
| 1:2:1328:A:H62   | 1:2:1489:C:H42   | 1.65                     | 0.43              |
| 1:2:1535:G:C6    | 1:2:1589:A:N1    | 2.87                     | 0.43              |
| 1:2:1707:A:H2'   | 1:2:1708:C:H6    | 1.83                     | 0.43              |
| 3:D:85:LYS:N     | 3:D:102:GLY:O    | 2.42                     | 0.43              |
| 3:D:195:LYS:HD3  | 3:D:195:LYS:HA   | 1.85                     | 0.43              |
| 5:F:55:THR:HA    | 5:F:58:VAL:HB    | 2.01                     | 0.43              |
| 5:F:162:ASP:O    | 5:F:164:VAL:N    | 2.52                     | 0.43              |
| 9:J:143:ARG:HH22 | 24:Y:53:ILE:HA   | 1.83                     | 0.43              |
| 12:M:5:LYS:HG3   | 12:M:6:LYS:HD3   | 2.00                     | 0.43              |
| 18:S:76:GLY:O    | 18:S:80:GLN:N    | 2.42                     | 0.43              |
| 24:Y:49:GLU:CD   | 24:Y:50:PHE:H    | 2.26                     | 0.43              |
| 28:c:30:SER:HB2  | 28:c:48:SER:OG   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:348:C:H2'    | 1:2:349:U:C6      | 2.54                     | 0.42              |
| 1:2:559:A:H2'    | 1:2:560:C:C6      | 2.54                     | 0.42              |
| 1:2:740:G:H2'    | 1:2:741:C:C6      | 2.54                     | 0.42              |
| 1:2:1413:C:OP1   | 21:V:129:ARG:HD3  | 2.18                     | 0.42              |
| 1:2:1615:A:H8    | 17:R:40:ARG:NH2   | 2.16                     | 0.42              |
| 3:D:171:ILE:HG21 | 3:D:197:ILE:HG12  | 2.00                     | 0.42              |
| 3:D:227:LYS:HA   | 3:D:230:GLU:HB3   | 2.01                     | 0.42              |
| 4:E:119:ASN:O    | 4:E:152:ARG:NH2   | 2.26                     | 0.42              |
| 4:E:238:PRO:HA   | 4:E:241:TRP:CE2   | 2.54                     | 0.42              |
| 5:F:177:LEU:HD23 | 5:F:177:LEU:HA    | 1.90                     | 0.42              |
| 6:G:69:PHE:CD2   | 26:a:17:LEU:HD11  | 2.54                     | 0.42              |
| 6:G:127:ARG:HB2  | 6:G:140:VAL:HG12  | 2.00                     | 0.42              |
| 6:G:137:PRO:HD2  | 6:G:149:TYR:CD1   | 2.54                     | 0.42              |
| 19:T:50:ILE:O    | 19:T:54:VAL:HG23  | 2.19                     | 0.42              |
| 24:Y:73:GLY:HA3  | 24:Y:128:PHE:CZ   | 2.54                     | 0.42              |
| 32:g:19:THR:O    | 32:g:288:SER:HB3  | 2.18                     | 0.42              |
| 32:g:99:ARG:NH1  | 32:g:134:THR:O    | 2.52                     | 0.42              |
| 1:2:664:C:H42    | 1:2:1027:A:H61    | 1.67                     | 0.42              |
| 1:2:831:C:O5'    | 26:a:8:ARG:NH2    | 2.52                     | 0.42              |
| 1:2:1035:C:N4    | 1:2:1073:A:H61    | 2.17                     | 0.42              |
| 1:2:1103:G:H2'   | 1:2:1104:G:C8     | 2.54                     | 0.42              |
| 1:2:1404:U:H2'   | 1:2:1405:A:O4'    | 2.19                     | 0.42              |
| 1:2:1451:A:H61   | 1:2:1467:C:H42    | 1.66                     | 0.42              |
| 1:2:1653:G:H5''  | 30:e:33:LYS:HZ2   | 1.84                     | 0.42              |
| 3:D:129:THR:OG1  | 3:D:131:ASP:OD1   | 2.28                     | 0.42              |
| 3:D:140:VAL:N    | 3:D:211:PHE:O     | 2.36                     | 0.42              |
| 11:L:36:GLY:CA   | 11:L:123:ILE:HD12 | 2.49                     | 0.42              |
| 11:L:108:ARG:NE  | 11:L:154:GLN:HE22 | 2.18                     | 0.42              |
| 13:N:16:ILE:HG13 | 13:N:17:PHE:N     | 2.31                     | 0.42              |
| 17:R:76:VAL:O    | 17:R:95:GLY:N     | 2.38                     | 0.42              |
| 19:T:72:LYS:HD2  | 19:T:75:GLU:OE2   | 2.20                     | 0.42              |
| 19:T:80:ARG:HA   | 19:T:83:ASN:ND2   | 2.34                     | 0.42              |
| 19:T:122:PRO:HA  | 19:T:123:THR:HA   | 1.85                     | 0.42              |
| 20:U:24:ARG:HD3  | 20:U:25:LYS:H     | 1.84                     | 0.42              |
| 24:Y:80:ASP:OD1  | 24:Y:81:VAL:N     | 2.52                     | 0.42              |
| 27:b:75:VAL:O    | 27:b:79:ILE:HG22  | 2.19                     | 0.42              |
| 36:y:18:G:O5'    | 36:y:59:A:N6      | 2.52                     | 0.42              |
| 1:2:96:C:H1'     | 1:2:464:G:H5'     | 2.01                     | 0.42              |
| 1:2:792:G:O2'    | 1:2:793:C:O4'     | 2.33                     | 0.42              |
| 1:2:797:U:H2'    | 1:2:798:A:C8      | 2.54                     | 0.42              |
| 1:2:955:G:H2'    | 1:2:956:U:C6      | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:967:G:H4'    | 1:2:968:A:C8     | 2.54                     | 0.42              |
| 1:2:1095:G:H2'   | 1:2:1096:A:H8    | 1.84                     | 0.42              |
| 1:2:1236:A:H2'   | 1:2:1237:A:C8    | 2.54                     | 0.42              |
| 1:2:1309:A:H3'   | 14:O:92:CYS:SG   | 2.59                     | 0.42              |
| 1:2:1328:A:O2'   | 5:F:145:GLN:O    | 2.37                     | 0.42              |
| 1:2:1517:A:C8    | 17:R:128:HIS:CD2 | 3.07                     | 0.42              |
| 1:2:1766:C:H2'   | 1:2:1767:C:C6    | 2.54                     | 0.42              |
| 1:2:1860:A:H4'   | 27:b:95:ARG:HD2  | 2.02                     | 0.42              |
| 4:E:77:GLU:O     | 4:E:81:PHE:N     | 2.52                     | 0.42              |
| 4:E:177:LEU:HD23 | 4:E:177:LEU:H    | 1.84                     | 0.42              |
| 5:F:133:GLY:HA2  | 5:F:155:GLY:HA3  | 2.01                     | 0.42              |
| 6:G:132:GLY:N    | 6:G:136:ILE:O    | 2.36                     | 0.42              |
| 11:L:152:ASP:O   | 11:L:155:LYS:HG2 | 2.20                     | 0.42              |
| 1:2:236:C:H2'    | 1:2:237:G:C8     | 2.54                     | 0.42              |
| 1:2:882:A:C2     | 1:2:897:G:C4     | 3.08                     | 0.42              |
| 1:2:1386:U:C2    | 1:2:1387:C:C5    | 3.07                     | 0.42              |
| 1:2:1394:G:H2'   | 1:2:1395:C:H6    | 1.84                     | 0.42              |
| 1:2:1699:C:O2'   | 1:2:1700:C:H5'   | 2.20                     | 0.42              |
| 1:2:1769:U:H2'   | 1:2:1770:G:H8    | 1.83                     | 0.42              |
| 2:C:143:PRO:HB3  | 23:X:32:ILE:HD12 | 2.00                     | 0.42              |
| 4:E:168:LYS:HD2  | 4:E:179:ARG:CZ   | 2.49                     | 0.42              |
| 9:J:139:ILE:H    | 15:P:19:ARG:NH2  | 2.17                     | 0.42              |
| 9:J:144:ILE:HG22 | 9:J:154:ILE:HG23 | 2.02                     | 0.42              |
| 11:L:83:ARG:HD2  | 11:L:150:ARG:HG2 | 2.01                     | 0.42              |
| 15:P:38:TYR:O    | 15:P:42:LYS:HG3  | 2.19                     | 0.42              |
| 17:R:98:ASN:CG   | 17:R:99:GLY:H    | 2.26                     | 0.42              |
| 19:T:6:THR:O     | 19:T:10:LYS:HG2  | 2.19                     | 0.42              |
| 27:b:45:VAL:HG13 | 27:b:64:LEU:HD11 | 2.00                     | 0.42              |
| 34:i:89:GLN:OE1  | 34:i:89:GLN:N    | 2.52                     | 0.42              |
| 1:2:152:U:H2'    | 1:2:153:G:C8     | 2.54                     | 0.42              |
| 1:2:812:A:H2'    | 1:2:813:G:O4'    | 2.19                     | 0.42              |
| 1:2:839:C:H1'    | 6:G:263:GLY:H    | 1.84                     | 0.42              |
| 1:2:960:A:H2'    | 1:2:961:U:C6     | 2.54                     | 0.42              |
| 1:2:1222:G:O6    | 1:2:1636:A:N6    | 2.52                     | 0.42              |
| 1:2:1271:G:H1    | 1:2:1502:A:H2'   | 1.85                     | 0.42              |
| 1:2:1507:U:H2'   | 1:2:1508:C:C6    | 2.54                     | 0.42              |
| 1:2:1697:G:C5    | 1:2:1698:C:C4    | 3.08                     | 0.42              |
| 3:D:33:VAL:HA    | 3:D:96:CYS:HB2   | 2.00                     | 0.42              |
| 3:D:113:MET:HE1  | 3:D:211:PHE:CE2  | 2.54                     | 0.42              |
| 4:E:233:TYR:OH   | 23:X:12:TYR:O    | 2.36                     | 0.42              |
| 6:G:104:ASP:N    | 6:G:108:ARG:O    | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:H:38:TYR:CD1    | 7:H:144:LEU:HD13  | 2.54                     | 0.42              |
| 8:I:170:ARG:HD3   | 8:I:172:LYS:HG2   | 2.00                     | 0.42              |
| 10:K:195:LEU:O    | 10:K:199:LEU:HD23 | 2.20                     | 0.42              |
| 18:S:40:GLU:O     | 18:S:48:GLN:NE2   | 2.52                     | 0.42              |
| 20:U:23:ARG:HH12  | 33:h:48:VAL:H     | 1.68                     | 0.42              |
| 20:U:80:PRO:HB2   | 20:U:82:TRP:HE1   | 1.84                     | 0.42              |
| 20:U:89:ASP:O     | 20:U:90:VAL:HG23  | 2.19                     | 0.42              |
| 35:l:20:MET:O     | 35:l:23:ARG:HG2   | 2.19                     | 0.42              |
| 1:2:51:U:C2       | 1:2:52:G:N7       | 2.88                     | 0.42              |
| 1:2:682:G:C6      | 1:2:733:G:N1      | 2.88                     | 0.42              |
| 1:2:826:A:C6      | 1:2:841:G:N1      | 2.88                     | 0.42              |
| 1:2:1226:C:H1'    | 1:2:1660:G:H22    | 1.84                     | 0.42              |
| 1:2:1352:G:O3'    | 4:E:110:LYS:NZ    | 2.52                     | 0.42              |
| 2:C:87:VAL:HG12   | 2:C:175:TRP:CH2   | 2.54                     | 0.42              |
| 2:C:124:VAL:O     | 2:C:146:ALA:HA    | 2.19                     | 0.42              |
| 3:D:225:LEU:HD23  | 3:D:228:LEU:HD13  | 2.01                     | 0.42              |
| 11:L:147:PHE:CD2  | 11:L:149:VAL:HG22 | 2.54                     | 0.42              |
| 13:N:81:LYS:HE2   | 13:N:81:LYS:HB3   | 1.87                     | 0.42              |
| 15:P:64:ARG:HD3   | 15:P:70:LYS:HG2   | 2.00                     | 0.42              |
| 17:R:59:ARG:HH21  | 17:R:76:VAL:HG13  | 1.84                     | 0.42              |
| 17:R:122:THR:HG23 | 17:R:123:TYR:HD1  | 1.84                     | 0.42              |
| 19:T:104:GLU:HA   | 19:T:107:LYS:HB3  | 2.00                     | 0.42              |
| 23:X:59:ILE:HD11  | 23:X:64:GLU:HB2   | 2.01                     | 0.42              |
| 25:Z:67:ARG:HD3   | 25:Z:67:ARG:HA    | 1.77                     | 0.42              |
| 29:d:17:VAL:HG23  | 29:d:30:VAL:HG22  | 2.01                     | 0.42              |
| 29:d:43:ILE:O     | 29:d:44:ARG:HD2   | 2.19                     | 0.42              |
| 31:f:111:ASN:HA   | 31:f:112:GLY:HA2  | 1.57                     | 0.42              |
| 37:z:547:G:C2     | 37:z:549:G:H8     | 2.37                     | 0.42              |
| 37:z:561:U:H2'    | 37:z:562:G:O4'    | 2.20                     | 0.42              |
| 1:2:376:C:OP2     | 13:N:136:LYS:NZ   | 2.35                     | 0.42              |
| 1:2:432:C:H2'     | 1:2:433:U:C6      | 2.54                     | 0.42              |
| 1:2:565:A:OP1     | 26:a:93:ARG:NH2   | 2.52                     | 0.42              |
| 1:2:839:C:H2'     | 1:2:840:U:C6      | 2.55                     | 0.42              |
| 1:2:1187:C:H2'    | 1:2:1188:U:C6     | 2.54                     | 0.42              |
| 1:2:1228:U:H2'    | 1:2:1229:G:C8     | 2.54                     | 0.42              |
| 1:2:1236:A:N3     | 17:R:100:LYS:HE2  | 2.35                     | 0.42              |
| 1:2:1561:G:OP2    | 21:V:101:ARG:NH2  | 2.45                     | 0.42              |
| 1:2:1640:C:H5''   | 18:S:138:ARG:CZ   | 2.50                     | 0.42              |
| 1:2:1767:C:H2'    | 1:2:1768:C:H6     | 1.84                     | 0.42              |
| 2:C:31:ASP:OD1    | 2:C:32:PHE:N      | 2.52                     | 0.42              |
| 2:C:53:ARG:NH1    | 23:X:82:ASN:OD1   | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:E:92:LEU:HB2   | 4:E:112:PHE:HB2  | 2.00                     | 0.42              |
| 6:G:6:LYS:HG2    | 6:G:30:ARG:HH12  | 1.83                     | 0.42              |
| 12:M:14:LEU:HA   | 12:M:17:LYS:HG2  | 2.02                     | 0.42              |
| 14:O:46:GLN:HE22 | 14:O:112:LYS:HB3 | 1.85                     | 0.42              |
| 17:R:10:ARG:HA   | 17:R:10:ARG:HD2  | 1.75                     | 0.42              |
| 17:R:39:ALA:HA   | 17:R:42:ARG:HE   | 1.84                     | 0.42              |
| 33:h:103:HIS:CG  | 33:h:104:ARG:N   | 2.87                     | 0.42              |
| 36:y:8:U:O3'     | 36:y:9:G:H3'     | 2.19                     | 0.42              |
| 1:2:8:U:O2'      | 1:2:9:U:H5'      | 2.19                     | 0.42              |
| 1:2:144:U:H2'    | 1:2:145:G:H8     | 1.83                     | 0.42              |
| 1:2:865:A:C4     | 1:2:911:G:H1'    | 2.55                     | 0.42              |
| 1:2:882:A:H61    | 1:2:896:C:N4     | 2.15                     | 0.42              |
| 1:2:1014:U:H2'   | 1:2:1015:C:C6    | 2.54                     | 0.42              |
| 1:2:1233:C:H4'   | 17:R:128:HIS:HE1 | 1.85                     | 0.42              |
| 1:2:1237:A:H2    | 1:2:1511:G:H21   | 1.66                     | 0.42              |
| 1:2:1301:C:H5'   | 31:f:92:LYS:NZ   | 2.35                     | 0.42              |
| 1:2:1327:C:H4'   | 1:2:1328:A:C5'   | 2.49                     | 0.42              |
| 1:2:1351:C:O2    | 4:E:220:ASN:ND2  | 2.53                     | 0.42              |
| 1:2:1611:U:H2'   | 1:2:1612:G:O4'   | 2.20                     | 0.42              |
| 2:C:105:PRO:CB   | 2:C:132:GLN:HE21 | 2.33                     | 0.42              |
| 4:E:93:LYS:HD3   | 4:E:95:MET:SD    | 2.60                     | 0.42              |
| 7:H:140:ASP:OD2  | 29:d:58:LEU:HG   | 2.20                     | 0.42              |
| 11:L:122:SER:OG  | 11:L:123:ILE:N   | 2.53                     | 0.42              |
| 15:P:38:TYR:CD1  | 15:P:78:LYS:HE2  | 2.54                     | 0.42              |
| 21:V:6:VAL:HA    | 21:V:9:VAL:HG22  | 2.02                     | 0.42              |
| 22:W:31:SER:O    | 22:W:35:VAL:HG23 | 2.20                     | 0.42              |
| 23:X:9:VAL:HG22  | 23:X:10:ASP:H    | 1.85                     | 0.42              |
| 29:d:44:ARG:HA   | 29:d:65:ALA:HB3  | 2.01                     | 0.42              |
| 1:2:157:U:H4'    | 8:I:59:GLN:HA    | 2.02                     | 0.42              |
| 1:2:348:C:C2     | 1:2:395:G:C2     | 3.07                     | 0.42              |
| 1:2:360:G:N2     | 1:2:362:U:O4     | 2.52                     | 0.42              |
| 1:2:517:C:OP1    | 11:L:125:HIS:N   | 2.52                     | 0.42              |
| 1:2:561:U:H2'    | 1:2:562:U:C6     | 2.55                     | 0.42              |
| 1:2:1088:G:N1    | 1:2:1154:G:O6    | 2.53                     | 0.42              |
| 1:2:1105:C:C6    | 19:T:122:PRO:HB3 | 2.55                     | 0.42              |
| 1:2:1251:G:OP1   | 1:2:1252:G:O2'   | 2.33                     | 0.42              |
| 1:2:1260:C:O2    | 1:2:1512:G:N2    | 2.50                     | 0.42              |
| 1:2:1413:C:H2'   | 1:2:1415:C:C6    | 2.55                     | 0.42              |
| 1:2:1535:G:C2    | 1:2:1536:G:C5    | 3.08                     | 0.42              |
| 1:2:1848:U:H2'   | 1:2:1849:G:H8    | 1.84                     | 0.42              |
| 25:Z:135:LYS:HD2 | 25:Z:135:LYS:HA  | 1.89                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:a:88:LYS:HA    | 26:a:91:LEU:HD12  | 2.01                     | 0.42              |
| 33:h:106:GLN:HE22 | 33:h:108:ILE:CD1  | 2.30                     | 0.42              |
| 1:2:1068:U:H5''   | 1:2:1069:U:OP2    | 2.20                     | 0.42              |
| 1:2:1436:C:H2'    | 1:2:1437:U:C6     | 2.55                     | 0.42              |
| 1:2:1482:A:H2'    | 1:2:1483:A:O4'    | 2.20                     | 0.42              |
| 1:2:1553:C:H2'    | 1:2:1554:C:H6     | 1.84                     | 0.42              |
| 1:2:1795:A:H2'    | 1:2:1796:C:H6     | 1.84                     | 0.42              |
| 1:2:1860:A:N6     | 27:b:87:ARG:HD2   | 2.35                     | 0.42              |
| 4:E:45:TRP:CZ3    | 4:E:56:LYS:HD3    | 2.55                     | 0.42              |
| 6:G:165:GLU:OE1   | 6:G:165:GLU:N     | 2.52                     | 0.42              |
| 9:J:58:LYS:HD2    | 9:J:58:LYS:HA     | 1.93                     | 0.42              |
| 9:J:157:HIS:HA    | 9:J:188:GLU:O     | 2.20                     | 0.42              |
| 9:J:177:TYR:CE2   | 9:J:183:LYS:HB2   | 2.55                     | 0.42              |
| 15:P:100:LYS:HA   | 15:P:103:GLU:HG2  | 2.02                     | 0.42              |
| 17:R:79:HIS:CE1   | 17:R:102:PHE:HZ   | 2.37                     | 0.42              |
| 17:R:106:GLU:OE2  | 17:R:107:ILE:N    | 2.53                     | 0.42              |
| 20:U:103:LEU:O    | 20:U:107:LEU:N    | 2.52                     | 0.42              |
| 22:W:36:CYS:SG    | 22:W:53:PRO:HB3   | 2.59                     | 0.42              |
| 26:a:22:GLN:HB2   | 26:a:72:PHE:CZ    | 2.54                     | 0.42              |
| 32:g:206:LEU:HD13 | 32:g:227:LEU:HD12 | 2.01                     | 0.42              |
| 36:y:38:C:H3'     | 36:y:39:C:C6      | 2.55                     | 0.42              |
| 1:2:81:U:H2'      | 1:2:82:G:O4'      | 2.19                     | 0.41              |
| 1:2:163:U:OP1     | 8:I:85:ARG:N      | 2.53                     | 0.41              |
| 1:2:872:C:O2'     | 1:2:873:C:O2      | 2.26                     | 0.41              |
| 1:2:1573:U:N3     | 5:F:1:MET:O       | 2.53                     | 0.41              |
| 1:2:1622:C:O3'    | 21:V:41:LYS:HD2   | 2.20                     | 0.41              |
| 1:2:1858:U:H3'    | 27:b:5:ARG:NH2    | 2.35                     | 0.41              |
| 4:E:51:LEU:O      | 4:E:55:VAL:HG23   | 2.20                     | 0.41              |
| 4:E:57:ASP:OD2    | 4:E:257:HIS:ND1   | 2.53                     | 0.41              |
| 5:F:203:PRO:HG3   | 19:T:42:PRO:HB2   | 2.02                     | 0.41              |
| 6:G:182:MET:HB3   | 6:G:226:PHE:HB3   | 2.02                     | 0.41              |
| 9:J:70:LYS:O      | 9:J:74:LYS:HG3    | 2.18                     | 0.41              |
| 9:J:100:ILE:HG22  | 9:J:125:VAL:HG21  | 2.02                     | 0.41              |
| 11:L:18:ARG:O     | 11:L:24:ARG:NH1   | 2.53                     | 0.41              |
| 12:M:42:ASN:C     | 12:M:44:HIS:H     | 2.27                     | 0.41              |
| 15:P:142:GLU:OE1  | 15:P:144:SER:N    | 2.46                     | 0.41              |
| 17:R:17:TYR:HA    | 20:U:91:LYS:HG2   | 2.01                     | 0.41              |
| 23:X:42:VAL:HG23  | 23:X:43:THR:HG23  | 2.01                     | 0.41              |
| 24:Y:30:CYS:SG    | 24:Y:61:ILE:N     | 2.90                     | 0.41              |
| 26:a:111:LYS:O    | 26:a:115:LYS:HG3  | 2.20                     | 0.41              |
| 29:d:16:LYS:HA    | 29:d:16:LYS:HD2   | 1.79                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 32:g:241:PHE:CE1 | 32:g:248:LEU:HD13 | 2.55                     | 0.41              |
| 1:2:40:A:H2'     | 1:2:476:A:N7      | 2.35                     | 0.41              |
| 1:2:377:C:H2'    | 1:2:378:U:C6      | 2.54                     | 0.41              |
| 1:2:465:C:H2'    | 1:2:497:G:H21     | 1.85                     | 0.41              |
| 1:2:1006:G:H2'   | 1:2:1007:A:C8     | 2.53                     | 0.41              |
| 1:2:1184:A:H2'   | 1:2:1185:A:O4'    | 2.21                     | 0.41              |
| 1:2:1453:U:C2    | 1:2:1454:G:N7     | 2.88                     | 0.41              |
| 1:2:1652:G:C2    | 1:2:1653:G:C5     | 3.08                     | 0.41              |
| 2:C:83:GLY:O     | 2:C:87:VAL:HG22   | 2.20                     | 0.41              |
| 3:D:173:THR:O    | 3:D:177:GLN:HG3   | 2.20                     | 0.41              |
| 4:E:179:ARG:O    | 4:E:209:THR:HA    | 2.20                     | 0.41              |
| 6:G:112:HIS:HE1  | 6:G:239:PRO:HG3   | 1.85                     | 0.41              |
| 14:O:58:GLU:HG3  | 14:O:61:TYR:H     | 1.85                     | 0.41              |
| 15:P:47:PRO:HA   | 15:P:50:ILE:HD12  | 2.00                     | 0.41              |
| 15:P:98:VAL:HG11 | 15:P:115:LEU:HB2  | 2.02                     | 0.41              |
| 16:Q:124:MET:HA  | 16:Q:124:MET:HE3  | 2.02                     | 0.41              |
| 21:V:51:ASN:HB3  | 21:V:54:TYR:HD2   | 1.86                     | 0.41              |
| 24:Y:15:ASN:O    | 24:Y:19:LYS:HG3   | 2.19                     | 0.41              |
| 24:Y:115:GLU:CD  | 24:Y:118:ARG:HH12 | 2.28                     | 0.41              |
| 25:Z:21:LYS:NZ   | 25:Z:27:TYR:CZ    | 2.83                     | 0.41              |
| 32:g:291:TRP:CZ3 | 32:g:298:LEU:HB3  | 2.56                     | 0.41              |
| 37:z:575:A:C8    | 37:z:576:C:H4'    | 2.47                     | 0.41              |
| 1:2:167:G:N1     | 1:2:168:C:N4      | 2.68                     | 0.41              |
| 1:2:348:C:H2'    | 1:2:349:U:H6      | 1.84                     | 0.41              |
| 1:2:512:A:H5''   | 11:L:145:PRO:HD2  | 2.02                     | 0.41              |
| 1:2:649:G:O2'    | 1:2:652:G:O2'     | 2.20                     | 0.41              |
| 1:2:1120:C:H2'   | 1:2:1121:C:C6     | 2.55                     | 0.41              |
| 1:2:1192:A:C5    | 1:2:1193:G:C8     | 3.08                     | 0.41              |
| 1:2:1328:A:N1    | 1:2:1496:G:C5     | 2.88                     | 0.41              |
| 1:2:1498:C:H2'   | 1:2:1499:C:H6     | 1.85                     | 0.41              |
| 1:2:1833:U:H5'   | 16:Q:150:ARG:CZ   | 2.50                     | 0.41              |
| 2:C:199:PRO:HG2  | 19:T:91:LEU:CD1   | 2.50                     | 0.41              |
| 5:F:51:LEU:HD12  | 5:F:89:GLU:OE2    | 2.21                     | 0.41              |
| 8:I:62:PRO:O     | 8:I:63:MET:HE2    | 2.19                     | 0.41              |
| 10:K:67:TRP:HE1  | 13:N:20:LYS:NZ    | 2.19                     | 0.41              |
| 13:N:80:MET:SD   | 13:N:86:ILE:HA    | 2.60                     | 0.41              |
| 13:N:147:LYS:HD2 | 13:N:147:LYS:HA   | 1.81                     | 0.41              |
| 15:P:26:LEU:H    | 15:P:26:LEU:HD12  | 1.85                     | 0.41              |
| 16:Q:142:ARG:NH2 | 27:b:22:ARG:HB3   | 2.32                     | 0.41              |
| 18:S:8:GLN:HB2   | 18:S:27:ARG:HB2   | 2.02                     | 0.41              |
| 18:S:85:ARG:HH22 | 18:S:117:ARG:HB3  | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:a:109:GLU:O    | 26:a:113:ARG:HG2  | 2.20                     | 0.41              |
| 32:g:130:LYS:HA   | 32:g:141:THR:HA   | 2.03                     | 0.41              |
| 1:2:74:G:O6       | 8:I:170:ARG:NH2   | 2.53                     | 0.41              |
| 1:2:516:A:H5''    | 34:i:109:ARG:HH12 | 1.85                     | 0.41              |
| 1:2:560:C:C2      | 1:2:561:U:C5      | 3.08                     | 0.41              |
| 1:2:656:U:H2'     | 1:2:657:U:C6      | 2.56                     | 0.41              |
| 1:2:1030:A:C2     | 1:2:1031:A:H1'    | 2.55                     | 0.41              |
| 1:2:1180:G:H2'    | 1:2:1181:C:C6     | 2.56                     | 0.41              |
| 1:2:1431:C:H4'    | 1:2:1432:C:OP1    | 2.21                     | 0.41              |
| 1:2:1721:G:H2'    | 1:2:1722:G:C8     | 2.56                     | 0.41              |
| 1:2:1734:C:H2'    | 1:2:1735:C:H6     | 1.86                     | 0.41              |
| 1:2:1814:G:H2'    | 1:2:1815:U:C6     | 2.55                     | 0.41              |
| 5:F:18:LYS:HB3    | 30:e:50:ILE:HG21  | 2.01                     | 0.41              |
| 15:P:29:THR:O     | 15:P:33:VAL:HG23  | 2.20                     | 0.41              |
| 17:R:33:LEU:HD21  | 17:R:86:LEU:HD22  | 2.03                     | 0.41              |
| 32:g:302:TYR:HB2  | 32:g:304:ASP:OD1  | 2.21                     | 0.41              |
| 36:y:8:U:O2'      | 36:y:10:G:OP1     | 2.24                     | 0.41              |
| 36:y:29:G:H2'     | 36:y:30:G:H8      | 1.80                     | 0.41              |
| 37:z:579:G:C6     | 37:z:590:A:C6     | 3.08                     | 0.41              |
| 1:2:85:A:H5''     | 26:a:118:ARG:NH1  | 2.35                     | 0.41              |
| 1:2:92:A:C8       | 1:2:437:A:C4      | 3.09                     | 0.41              |
| 1:2:108:G:C6      | 1:2:109:U:N3      | 2.88                     | 0.41              |
| 1:2:376:C:H4'     | 10:K:9:HIS:HE1    | 1.85                     | 0.41              |
| 1:2:553:G:O2'     | 1:2:554:A:O5'     | 2.37                     | 0.41              |
| 1:2:585:U:H2'     | 1:2:586:U:C6      | 2.55                     | 0.41              |
| 1:2:625:G:H2'     | 1:2:626:C:H6      | 1.85                     | 0.41              |
| 1:2:796:U:H2'     | 1:2:797:U:O4'     | 2.20                     | 0.41              |
| 1:2:837:G:H2'     | 1:2:838:C:H6      | 1.84                     | 0.41              |
| 1:2:1816:A:H2'    | 1:2:1817:A:C8     | 2.55                     | 0.41              |
| 6:G:182:MET:HE2   | 6:G:182:MET:HA    | 2.02                     | 0.41              |
| 9:J:153:LEU:HD21  | 9:J:186:ASN:HB2   | 2.02                     | 0.41              |
| 18:S:32:ILE:O     | 18:S:39:LEU:HD22  | 2.20                     | 0.41              |
| 24:Y:103:VAL:HG13 | 24:Y:126:LEU:HB2  | 2.02                     | 0.41              |
| 27:b:41:ILE:O     | 27:b:42:ARG:NH1   | 2.54                     | 0.41              |
| 30:e:23:VAL:HG13  | 30:e:38:MET:SD    | 2.60                     | 0.41              |
| 34:i:114:ARG:HA   | 34:i:114:ARG:HD2  | 1.80                     | 0.41              |
| 36:y:27:U:C2      | 36:y:42:G:N2      | 2.88                     | 0.41              |
| 1:2:102:A:OP2     | 10:K:19:LYS:NZ    | 2.39                     | 0.41              |
| 1:2:412:U:H2'     | 1:2:413:U:C6      | 2.55                     | 0.41              |
| 1:2:569:C:H2'     | 1:2:570:U:O4'     | 2.20                     | 0.41              |
| 1:2:637:U:C2      | 1:2:638:A:C8      | 3.08                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:820:C:C2     | 11:L:144:ILE:HG13 | 2.55                     | 0.41              |
| 1:2:905:G:C2     | 1:2:906:G:C5      | 3.09                     | 0.41              |
| 1:2:1060:C:O3'   | 16:Q:149:ARG:NH1  | 2.53                     | 0.41              |
| 1:2:1383:G:H3'   | 1:2:1384:A:H8     | 1.85                     | 0.41              |
| 1:2:1717:G:H2'   | 1:2:1718:G:C8     | 2.56                     | 0.41              |
| 1:2:1834:U:H2'   | 1:2:1835:C:C6     | 2.55                     | 0.41              |
| 2:C:184:ARG:HA   | 2:C:190:SER:HB3   | 2.01                     | 0.41              |
| 4:E:236:LEU:H    | 4:E:236:LEU:HD23  | 1.86                     | 0.41              |
| 7:H:63:LYS:HB3   | 7:H:63:LYS:HE2    | 1.81                     | 0.41              |
| 7:H:85:LYS:HD3   | 7:H:88:MET:SD     | 2.61                     | 0.41              |
| 9:J:104:PRO:HD3  | 9:J:116:ARG:HH11  | 1.85                     | 0.41              |
| 14:O:53:ALA:HA   | 14:O:79:VAL:O     | 2.21                     | 0.41              |
| 15:P:62:GLN:OE1  | 15:P:63:VAL:N     | 2.53                     | 0.41              |
| 15:P:113:PHE:O   | 15:P:117:LEU:HG   | 2.19                     | 0.41              |
| 26:a:20:ARG:HD2  | 26:a:76:TYR:CZ    | 2.55                     | 0.41              |
| 31:f:95:ARG:HH21 | 31:f:98:VAL:HG21  | 1.86                     | 0.41              |
| 32:g:22:ALA:HB3  | 32:g:32:LEU:HD12  | 2.01                     | 0.41              |
| 32:g:36:ARG:HG2  | 32:g:65:PHE:HB3   | 2.03                     | 0.41              |
| 32:g:177:TRP:HA  | 32:g:183:LYS:O    | 2.20                     | 0.41              |
| 36:y:16:C:O2     | 36:y:58:A:N6      | 2.54                     | 0.41              |
| 1:2:368:U:H2'    | 1:2:369:C:O4'     | 2.21                     | 0.41              |
| 1:2:559:A:H2'    | 1:2:560:C:H6      | 1.84                     | 0.41              |
| 1:2:1275:C:H2'   | 1:2:1276:G:C8     | 2.55                     | 0.41              |
| 1:2:1588:C:H2'   | 1:2:1589:A:C8     | 2.56                     | 0.41              |
| 1:2:1766:C:H2'   | 1:2:1767:C:H6     | 1.86                     | 0.41              |
| 1:2:1828:A:H2    | 1:2:1831:G:N1     | 2.19                     | 0.41              |
| 3:D:212:VAL:HG13 | 3:D:212:VAL:O     | 2.20                     | 0.41              |
| 6:G:91:SER:HA    | 6:G:98:ASN:OD1    | 2.19                     | 0.41              |
| 9:J:139:ILE:HD12 | 9:J:156:VAL:HG13  | 2.03                     | 0.41              |
| 11:L:75:ASN:HA   | 11:L:78:LEU:HG    | 2.02                     | 0.41              |
| 13:N:55:TYR:OH   | 13:N:116:CYS:HB2  | 2.20                     | 0.41              |
| 15:P:101:HIS:NE2 | 15:P:108:ASP:OD2  | 2.54                     | 0.41              |
| 20:U:34:LYS:HB3  | 20:U:100:ALA:HA   | 2.03                     | 0.41              |
| 20:U:65:GLU:O    | 20:U:69:THR:HG23  | 2.21                     | 0.41              |
| 23:X:15:ARG:NH1  | 23:X:33:PRO:HG3   | 2.36                     | 0.41              |
| 30:e:4:GLN:NE2   | 30:e:5:GLN:HB2    | 2.34                     | 0.41              |
| 37:z:568:A:H3'   | 37:z:569:A:H8     | 1.86                     | 0.41              |
| 37:z:592:C:C2    | 37:z:593:U:C5     | 3.09                     | 0.41              |
| 1:2:741:C:H2'    | 1:2:742:C:O4'     | 2.21                     | 0.41              |
| 1:2:987:G:H1'    | 27:b:11:ALA:HA    | 2.02                     | 0.41              |
| 1:2:1013:U:H2'   | 1:2:1014:U:C6     | 2.54                     | 0.41              |

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| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:2:1239:U:H2'  | 1:2:1240:U:O4'    | 2.21                     | 0.41              |
| 1:2:1281:G:H21  | 31:f:101:ALA:C    | 2.29                     | 0.41              |
| 1:2:1491:G:H22  | 30:e:45:GLN:CD    | 2.27                     | 0.41              |
| 1:2:1615:A:H1'  | 1:2:1619:U:OP2    | 2.21                     | 0.41              |
| 1:2:1660:G:C5   | 21:V:88:MET:HE1   | 2.56                     | 0.41              |
| 1:2:1721:G:C6   | 1:2:1803:A:C6     | 3.08                     | 0.41              |
| 1:2:1811:G:H2'  | 1:2:1812:A:C8     | 2.56                     | 0.41              |
| 4:E:98:GLN:HB3  | 4:E:107:THR:HG22  | 2.01                     | 0.41              |
| 4:E:155:TRP:H   | 4:E:163:HIS:CE1   | 2.38                     | 0.41              |
| 6:G:72:ILE:HD11 | 6:G:88:ASP:HB3    | 2.02                     | 0.41              |
| 6:G:122:LYS:HE3 | 6:G:143:ASP:OD2   | 2.20                     | 0.41              |
| 11:L:18:ARG:HD3 | 11:L:18:ARG:HA    | 1.82                     | 0.41              |
| 19:T:58:MET:SD  | 19:T:61:ILE:HD11  | 2.61                     | 0.41              |
| 25:Z:21:LYS:O   | 25:Z:21:LYS:HD3   | 2.20                     | 0.41              |
| 26:a:15:ASN:ND2 | 26:a:20:ARG:HE    | 2.19                     | 0.41              |
| 33:h:98:LYS:O   | 33:h:110:THR:HG22 | 2.19                     | 0.41              |
| 36:y:49:A:H4'   | 37:z:551:C:O3'    | 2.20                     | 0.41              |
| 37:z:584:A:H4'  | 37:z:585:G:C5     | 2.56                     | 0.41              |
| 1:2:67:C:H41    | 1:2:151:C:H4'     | 1.86                     | 0.41              |
| 1:2:152:U:H2'   | 1:2:153:G:O4'     | 2.21                     | 0.41              |
| 1:2:487:C:H2'   | 1:2:488:C:C6      | 2.56                     | 0.41              |
| 1:2:539:C:H2'   | 1:2:540:C:O4'     | 2.20                     | 0.41              |
| 1:2:551:A:OP2   | 11:L:174:LYS:N    | 2.34                     | 0.41              |
| 1:2:742:C:H2'   | 1:2:743:U:C5      | 2.55                     | 0.41              |
| 1:2:743:U:O2'   | 1:2:744:C:O4'     | 2.27                     | 0.41              |
| 1:2:746:C:H2'   | 1:2:747:G:C8      | 2.56                     | 0.41              |
| 1:2:820:C:H5'   | 11:L:147:PHE:CD1  | 2.56                     | 0.41              |
| 1:2:921:G:C2    | 1:2:922:A:C8      | 3.09                     | 0.41              |
| 1:2:959:A:P     | 16:Q:66:ARG:HB3   | 2.61                     | 0.41              |
| 1:2:1007:A:O3'  | 15:P:3:ARG:NH2    | 2.54                     | 0.41              |
| 1:2:1280:A:OP2  | 14:O:104:VAL:HG21 | 2.19                     | 0.41              |
| 1:2:1301:C:H5'  | 31:f:92:LYS:HZ3   | 1.86                     | 0.41              |
| 1:2:1331:G:H2'  | 1:2:1332:C:O4'    | 2.21                     | 0.41              |
| 1:2:1491:G:H2'  | 1:2:1492:U:C6     | 2.56                     | 0.41              |
| 1:2:1528:A:OP1  | 7:H:164:ARG:NH2   | 2.53                     | 0.41              |
| 1:2:1540:A:O5'  | 18:S:74:GLY:HA2   | 2.21                     | 0.41              |
| 1:2:1568:G:H2'  | 1:2:1569:C:C6     | 2.56                     | 0.41              |
| 1:2:1573:U:O2'  | 5:F:1:MET:N       | 2.54                     | 0.41              |
| 1:2:1586:C:O2'  | 7:H:87:LEU:HD23   | 2.21                     | 0.41              |
| 1:2:1589:A:C6   | 1:2:1590:U:C5     | 3.08                     | 0.41              |
| 1:2:1667:U:H2'  | 1:2:1668:U:C6     | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1695:C:C2     | 1:2:1828:A:N6     | 2.89                     | 0.41              |
| 2:C:38:ILE:HD12   | 2:C:38:ILE:HA     | 1.82                     | 0.41              |
| 2:C:198:MET:SD    | 2:C:199:PRO:HD2   | 2.61                     | 0.41              |
| 3:D:144:LYS:HD3   | 3:D:208:HIS:CG    | 2.56                     | 0.41              |
| 4:E:118:TYR:CE1   | 4:E:201:MET:HA    | 2.56                     | 0.41              |
| 4:E:255:THR:HA    | 4:E:258:LEU:HD12  | 2.03                     | 0.41              |
| 6:G:94:LYS:O      | 26:a:16:ARG:NH2   | 2.54                     | 0.41              |
| 8:I:30:LYS:O      | 8:I:101:ILE:HA    | 2.20                     | 0.41              |
| 9:J:64:VAL:HG22   | 9:J:96:ALA:HA     | 2.03                     | 0.41              |
| 9:J:157:HIS:HB3   | 9:J:190:PRO:HG3   | 2.03                     | 0.41              |
| 10:K:143:LYS:O    | 10:K:144:LYS:HB2  | 2.21                     | 0.41              |
| 11:L:172:ARG:HD3  | 11:L:172:ARG:HA   | 1.74                     | 0.41              |
| 12:M:15:LEU:HD22  | 12:M:49:MET:HE1   | 2.02                     | 0.41              |
| 12:M:29:MET:HA    | 12:M:30:PRO:HD3   | 1.94                     | 0.41              |
| 16:Q:103:ASN:HD21 | 16:Q:139:SER:HB2  | 1.86                     | 0.41              |
| 18:S:14:GLY:HA3   | 18:S:86:GLN:HE22  | 1.85                     | 0.41              |
| 21:V:52:TRP:HZ3   | 21:V:56:ARG:HE    | 1.69                     | 0.41              |
| 23:X:47:ASN:OD1   | 23:X:47:ASN:N     | 2.54                     | 0.41              |
| 26:a:74:MET:HE3   | 26:a:75:ILE:H     | 1.84                     | 0.41              |
| 29:d:60:GLU:HG2   | 29:d:62:GLU:H     | 1.85                     | 0.41              |
| 1:2:296:U:C2      | 10:K:55:TYR:HE2   | 2.39                     | 0.41              |
| 1:2:650:C:H2'     | 1:2:651:U:C6      | 2.56                     | 0.41              |
| 1:2:820:C:H2'     | 1:2:821:A:C8      | 2.56                     | 0.41              |
| 1:2:1026:A:H2'    | 1:2:1027:A:H8     | 1.85                     | 0.41              |
| 1:2:1211:C:N4     | 1:2:1216:A:H61    | 2.13                     | 0.41              |
| 1:2:1637:U:H2'    | 1:2:1638:U:H6     | 1.86                     | 0.41              |
| 1:2:1735:C:H2'    | 1:2:1736:U:C6     | 2.55                     | 0.41              |
| 1:2:1767:C:H2'    | 1:2:1768:C:C6     | 2.56                     | 0.41              |
| 1:2:1771:G:H2'    | 1:2:1772:C:C6     | 2.56                     | 0.41              |
| 1:2:1794:A:H2'    | 1:2:1795:A:O4'    | 2.21                     | 0.41              |
| 2:C:13:GLU:O      | 2:C:17:LYS:HG2    | 2.20                     | 0.41              |
| 5:F:121:GLY:HA2   | 5:F:124:ARG:HE    | 1.85                     | 0.41              |
| 7:H:178:ILE:HG22  | 7:H:182:LYS:NZ    | 2.36                     | 0.41              |
| 9:J:5:SER:HB3     | 9:J:8:ILE:HG12    | 2.03                     | 0.41              |
| 10:K:151:GLU:HB2  | 10:K:152:ARG:NH1  | 2.36                     | 0.41              |
| 11:L:110:LEU:HD21 | 11:L:142:VAL:HG21 | 2.02                     | 0.41              |
| 13:N:136:LYS:C    | 13:N:139:ARG:HH12 | 2.29                     | 0.41              |
| 16:Q:31:CYS:SG    | 16:Q:95:ILE:HG13  | 2.61                     | 0.41              |
| 21:V:71:GLY:O     | 21:V:74:SER:OG    | 2.32                     | 0.41              |
| 21:V:126:GLN:O    | 21:V:129:ARG:HB3  | 2.21                     | 0.41              |
| 25:Z:93:PHE:CD2   | 25:Z:133:LEU:HB3  | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 36:y:63:U:H2'    | 36:y:64:C:C6     | 2.55                     | 0.41              |
| 1:2:62:G:O2'     | 1:2:172:U:OP1    | 2.39                     | 0.40              |
| 1:2:487:C:H2'    | 1:2:488:C:H6     | 1.84                     | 0.40              |
| 1:2:673:G:N2     | 1:2:1018:U:OP2   | 2.54                     | 0.40              |
| 1:2:853:U:H2'    | 1:2:854:A:C8     | 2.57                     | 0.40              |
| 1:2:966:G:N2     | 1:2:966:G:OP1    | 2.54                     | 0.40              |
| 1:2:1061:G:OP2   | 16:Q:149:ARG:NH2 | 2.54                     | 0.40              |
| 1:2:1193:G:H2'   | 1:2:1194:G:C8    | 2.55                     | 0.40              |
| 1:2:1216:A:H2'   | 1:2:1217:G:O4'   | 2.22                     | 0.40              |
| 1:2:1294:G:C6    | 1:2:1295:A:C6    | 3.10                     | 0.40              |
| 1:2:1343:U:H2'   | 1:2:1344:G:C8    | 2.56                     | 0.40              |
| 1:2:1389:G:N2    | 1:2:1474:U:O4'   | 2.54                     | 0.40              |
| 1:2:1594:U:H5    | 7:H:165:ASN:C    | 2.28                     | 0.40              |
| 1:2:1618:A:O5'   | 20:U:133:GLY:HA3 | 2.21                     | 0.40              |
| 1:2:1732:G:C6    | 1:2:1791:U:O2    | 2.73                     | 0.40              |
| 1:2:1818:A:O2'   | 1:2:1819:A:H5''  | 2.21                     | 0.40              |
| 2:C:63:ARG:NH1   | 23:X:78:ILE:HD13 | 2.36                     | 0.40              |
| 2:C:140:VAL:HG12 | 2:C:140:VAL:O    | 2.20                     | 0.40              |
| 6:G:85:GLY:O     | 6:G:101:LEU:HD23 | 2.21                     | 0.40              |
| 7:H:65:GLN:OE1   | 7:H:65:GLN:N     | 2.53                     | 0.40              |
| 9:J:144:ILE:HG22 | 9:J:154:ILE:HG12 | 2.03                     | 0.40              |
| 11:L:91:LYS:HB3  | 11:L:96:TYR:HD2  | 1.84                     | 0.40              |
| 20:U:54:LYS:HB2  | 20:U:58:GLU:OE2  | 2.22                     | 0.40              |
| 21:V:41:LYS:HA   | 21:V:41:LYS:HD3  | 1.80                     | 0.40              |
| 26:a:78:SER:H    | 26:a:81:TYR:HD2  | 1.69                     | 0.40              |
| 27:b:4:LYS:HG2   | 27:b:5:ARG:HD2   | 2.03                     | 0.40              |
| 29:d:14:VAL:HG12 | 29:d:54:ASP:O    | 2.21                     | 0.40              |
| 29:d:21:THR:HG22 | 29:d:22:GLY:N    | 2.36                     | 0.40              |
| 29:d:45:ASN:OD1  | 29:d:65:ALA:HB1  | 2.21                     | 0.40              |
| 30:e:42:CYS:HA   | 30:e:45:GLN:HB2  | 2.04                     | 0.40              |
| 31:f:82:LYS:C    | 31:f:83:LYS:HD2  | 2.46                     | 0.40              |
| 32:g:101:PHE:CE1 | 32:g:136:GLY:HA2 | 2.56                     | 0.40              |
| 33:h:51:ASP:HB2  | 33:h:54:THR:HG23 | 2.02                     | 0.40              |
| 36:y:12:G:H2'    | 36:y:13:C:O4'    | 2.21                     | 0.40              |
| 36:y:50:U:H2'    | 36:y:51:G:C8     | 2.57                     | 0.40              |
| 37:z:571:A:C4    | 37:z:572:G:C8    | 3.09                     | 0.40              |
| 1:2:149:A:N7     | 1:2:169:U:O4     | 2.55                     | 0.40              |
| 1:2:499:G:H2'    | 1:2:500:G:C8     | 2.56                     | 0.40              |
| 1:2:813:G:N2     | 1:2:844:U:O4     | 2.54                     | 0.40              |
| 1:2:1093:G:H2'   | 1:2:1094:C:H6    | 1.86                     | 0.40              |
| 1:2:1139:A:H8    | 1:2:1139:A:OP1   | 2.04                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:1412:C:O2'    | 21:V:132:ASP:OD2 | 2.38                     | 0.40              |
| 1:2:1624:C:H5''   | 20:U:39:ARG:HG2  | 2.03                     | 0.40              |
| 1:2:1731:G:H2'    | 1:2:1732:G:H8    | 1.86                     | 0.40              |
| 2:C:63:ARG:CZ     | 23:X:78:ILE:HB   | 2.52                     | 0.40              |
| 5:F:212:GLU:OE2   | 19:T:38:ILE:HG13 | 2.21                     | 0.40              |
| 7:H:156:THR:HB    | 7:H:188:TYR:HE2  | 1.86                     | 0.40              |
| 19:T:31:ASN:C     | 19:T:31:ASN:HD22 | 2.29                     | 0.40              |
| 22:W:63:ILE:HB    | 22:W:80:PHE:HD2  | 1.86                     | 0.40              |
| 24:Y:50:PHE:HB2   | 24:Y:63:VAL:HG22 | 2.03                     | 0.40              |
| 31:f:102:VAL:HG13 | 31:f:103:LEU:N   | 2.36                     | 0.40              |
| 32:g:106:LYS:HB2  | 32:g:126:ASP:OD1 | 2.21                     | 0.40              |
| 32:g:191:HIS:CD2  | 32:g:217:MET:HG3 | 2.56                     | 0.40              |
| 1:2:523:A:H2'     | 1:2:524:G:C8     | 2.56                     | 0.40              |
| 1:2:888:U:H2'     | 1:2:889:U:C6     | 2.57                     | 0.40              |
| 1:2:1109:A:H2'    | 1:2:1110:U:C6    | 2.56                     | 0.40              |
| 1:2:1173:U:H2'    | 1:2:1174:U:H6    | 1.82                     | 0.40              |
| 1:2:1200:A:H2'    | 1:2:1201:C:C6    | 2.56                     | 0.40              |
| 1:2:1294:G:H5'    | 17:R:102:PHE:CZ  | 2.55                     | 0.40              |
| 1:2:1560:C:OP2    | 21:V:102:ARG:NH2 | 2.42                     | 0.40              |
| 1:2:1712:C:H2'    | 1:2:1713:G:O4'   | 2.22                     | 0.40              |
| 1:2:1786:G:H2'    | 1:2:1787:A:H8    | 1.87                     | 0.40              |
| 1:2:1788:C:H2'    | 1:2:1789:G:O4'   | 2.21                     | 0.40              |
| 1:2:1809:A:H3'    | 1:2:1810:G:H8    | 1.86                     | 0.40              |
| 5:F:94:ARG:HB2    | 5:F:125:PHE:HZ   | 1.86                     | 0.40              |
| 6:G:207:VAL:HG22  | 6:G:219:ALA:HB1  | 2.03                     | 0.40              |
| 8:I:2:LYS:O       | 8:I:108:VAL:HA   | 2.21                     | 0.40              |
| 8:I:54:GLY:O      | 8:I:110:ASN:N    | 2.53                     | 0.40              |
| 9:J:118:ARG:O     | 9:J:121:THR:HG22 | 2.21                     | 0.40              |
| 10:K:77:ARG:HD2   | 10:K:78:ILE:O    | 2.21                     | 0.40              |
| 10:K:197:PHE:O    | 10:K:200:ARG:HG2 | 2.21                     | 0.40              |
| 12:M:13:GLU:CD    | 12:M:83:LEU:HD13 | 2.47                     | 0.40              |
| 12:M:26:ASP:HB2   | 12:M:29:MET:HB2  | 2.04                     | 0.40              |
| 17:R:82:ASP:OD1   | 17:R:82:ASP:N    | 2.54                     | 0.40              |
| 17:R:85:ILE:HG21  | 17:R:111:MET:HB3 | 2.03                     | 0.40              |
| 20:U:81:ASP:OD1   | 20:U:81:ASP:N    | 2.55                     | 0.40              |
| 20:U:86:ARG:HD2   | 20:U:89:ASP:OD2  | 2.21                     | 0.40              |
| 26:a:124:ASN:OD1  | 26:a:124:ASN:N   | 2.53                     | 0.40              |
| 31:f:122:PRO:HD2  | 31:f:148:TYR:CZ  | 2.56                     | 0.40              |
| 35:l:3:ALA:HA     | 35:l:6:ARG:CZ    | 2.51                     | 0.40              |
| 35:l:5:TRP:CD1    | 35:l:5:TRP:N     | 2.88                     | 0.40              |
| 35:l:15:ARG:O     | 35:l:18:ARG:HG2  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:218:A:H2'    | 1:2:219:U:H6      | 1.86                     | 0.40              |
| 1:2:483:A:N6     | 1:2:499:G:H21     | 2.15                     | 0.40              |
| 1:2:560:C:H2'    | 1:2:561:U:H6      | 1.85                     | 0.40              |
| 1:2:845:A:H2'    | 1:2:846:C:C6      | 2.56                     | 0.40              |
| 1:2:860:A:H2'    | 1:2:861:A:C8      | 2.53                     | 0.40              |
| 1:2:1087:C:H2'   | 1:2:1088:G:C8     | 2.56                     | 0.40              |
| 1:2:1181:C:H2'   | 1:2:1182:U:C6     | 2.56                     | 0.40              |
| 1:2:1246:A:H4'   | 22:W:73:GLY:HA2   | 2.03                     | 0.40              |
| 1:2:1286:G:H2'   | 1:2:1287:A:O4'    | 2.21                     | 0.40              |
| 1:2:1372:A:P     | 19:T:67:ARG:HH12  | 2.44                     | 0.40              |
| 1:2:1805:C:H2'   | 1:2:1806:U:C6     | 2.57                     | 0.40              |
| 2:C:199:PRO:HB2  | 19:T:91:LEU:HD21  | 2.02                     | 0.40              |
| 3:D:31:TYR:CD1   | 3:D:94:LYS:HA     | 2.57                     | 0.40              |
| 4:E:151:ARG:HB2  | 4:E:233:TYR:CD2   | 2.54                     | 0.40              |
| 4:E:189:ILE:O    | 4:E:189:ILE:HG13  | 2.22                     | 0.40              |
| 6:G:45:ILE:CG2   | 6:G:80:ILE:HB     | 2.51                     | 0.40              |
| 6:G:125:LYS:NZ   | 6:G:225:ILE:O     | 2.44                     | 0.40              |
| 21:V:96:SER:HB2  | 21:V:99:VAL:HG22  | 2.03                     | 0.40              |
| 21:V:129:ARG:HG3 | 21:V:133:ARG:HH21 | 1.87                     | 0.40              |
| 37:z:584:A:H2'   | 37:z:586:A:C8     | 2.56                     | 0.40              |
| 1:2:50:A:H2'     | 1:2:51:U:O4'      | 2.22                     | 0.40              |
| 1:2:874:G:C2     | 1:2:905:G:C2      | 3.10                     | 0.40              |
| 1:2:971:G:C4     | 1:2:972:G:C8      | 3.10                     | 0.40              |
| 1:2:984:C:H5''   | 3:D:116:LYS:HG2   | 2.03                     | 0.40              |
| 1:2:1019:A:OP2   | 15:P:124:ARG:NH2  | 2.48                     | 0.40              |
| 1:2:1169:A:OP2   | 35:l:14:LYS:NZ    | 2.44                     | 0.40              |
| 1:2:1257:C:H2'   | 1:2:1258:C:O4'    | 2.22                     | 0.40              |
| 1:2:1643:G:H5''  | 18:S:125:ARG:CG   | 2.50                     | 0.40              |
| 5:F:99:ILE:H     | 5:F:99:ILE:HD12   | 1.86                     | 0.40              |
| 7:H:166:ILE:HD12 | 7:H:166:ILE:HA    | 1.94                     | 0.40              |
| 9:J:53:VAL:HG22  | 9:J:57:ARG:O      | 2.22                     | 0.40              |
| 9:J:160:LYS:HD2  | 9:J:189:PHE:CZ    | 2.56                     | 0.40              |
| 14:O:17:ALA:HA   | 14:O:124:ILE:HD12 | 2.04                     | 0.40              |
| 18:S:28:GLY:HA3  | 18:S:67:ASP:OD2   | 2.22                     | 0.40              |
| 25:Z:4:CYS:SG    | 25:Z:9:THR:HG21   | 2.61                     | 0.40              |
| 32:g:44:LYS:HG2  | 32:g:54:ILE:O     | 2.22                     | 0.40              |
| 32:g:170:TRP:HA  | 32:g:194:TYR:HB2  | 2.03                     | 0.40              |
| 32:g:191:HIS:CG  | 32:g:195:LEU:HD11 | 2.56                     | 0.40              |
| 37:z:523:G:H2'   | 37:z:524:C:H6     | 1.87                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2   | C     | 206/295 (70%) | 176 (85%) | 29 (14%) | 1 (0%)   | 24          | 63  |
| 3   | D     | 213/264 (81%) | 188 (88%) | 24 (11%) | 1 (0%)   | 24          | 63  |
| 4   | E     | 220/226 (97%) | 210 (96%) | 9 (4%)   | 1 (0%)   | 24          | 63  |
| 5   | F     | 225/243 (93%) | 211 (94%) | 13 (6%)  | 1 (0%)   | 30          | 67  |
| 6   | G     | 261/263 (99%) | 240 (92%) | 21 (8%)  | 0        | 100         | 100 |
| 7   | H     | 189/204 (93%) | 172 (91%) | 17 (9%)  | 0        | 100         | 100 |
| 8   | I     | 233/249 (94%) | 223 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 9   | J     | 188/194 (97%) | 174 (93%) | 14 (7%)  | 0        | 100         | 100 |
| 10  | K     | 204/208 (98%) | 177 (87%) | 23 (11%) | 4 (2%)   | 6           | 31  |
| 11  | L     | 180/194 (93%) | 173 (96%) | 6 (3%)   | 1 (1%)   | 21          | 58  |
| 12  | M     | 96/225 (43%)  | 83 (86%)  | 13 (14%) | 0        | 100         | 100 |
| 13  | N     | 156/158 (99%) | 149 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 14  | O     | 122/132 (92%) | 109 (89%) | 13 (11%) | 0        | 100         | 100 |
| 15  | P     | 148/151 (98%) | 144 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 16  | Q     | 134/168 (80%) | 115 (86%) | 19 (14%) | 0        | 100         | 100 |
| 17  | R     | 133/145 (92%) | 115 (86%) | 18 (14%) | 0        | 100         | 100 |
| 18  | S     | 139/146 (95%) | 133 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 19  | T     | 124/135 (92%) | 116 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 20  | U     | 140/152 (92%) | 123 (88%) | 16 (11%) | 1 (1%)   | 18          | 55  |
| 21  | V     | 139/141 (99%) | 127 (91%) | 11 (8%)  | 1 (1%)   | 18          | 55  |
| 22  | W     | 102/119 (86%) | 97 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 23  | X     | 80/83 (96%)   | 71 (89%)  | 9 (11%)  | 0        | 100         | 100 |
| 24  | Y     | 127/130 (98%) | 117 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 25  | Z     | 140/143 (98%) | 132 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 26  | a     | 122/126 (97%) | 111 (91%) | 9 (7%)   | 2 (2%)   | 7           | 37  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 27  | b     | 97/115 (84%)    | 88 (91%)   | 9 (9%)   | 0        | 100         | 100 |
| 28  | c     | 82/84 (98%)     | 74 (90%)   | 8 (10%)  | 0        | 100         | 100 |
| 29  | d     | 62/64 (97%)     | 60 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 30  | e     | 51/56 (91%)     | 41 (80%)   | 10 (20%) | 0        | 100         | 100 |
| 31  | f     | 69/156 (44%)    | 58 (84%)   | 11 (16%) | 0        | 100         | 100 |
| 32  | g     | 311/317 (98%)   | 285 (92%)  | 26 (8%)  | 0        | 100         | 100 |
| 33  | h     | 73/125 (58%)    | 70 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 34  | i     | 57/59 (97%)     | 52 (91%)   | 5 (9%)   | 0        | 100         | 100 |
| 35  | l     | 23/25 (92%)     | 23 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 4846/5495 (88%) | 4437 (92%) | 396 (8%) | 13 (0%)  | 37          | 71  |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | U     | 144 | ARG  |
| 5   | F     | 193 | ASP  |
| 10  | K     | 156 | ALA  |
| 26  | a     | 103 | SER  |
| 10  | K     | 144 | LYS  |
| 21  | V     | 40  | ALA  |
| 2   | C     | 206 | ASP  |
| 3   | D     | 207 | LEU  |
| 10  | K     | 52  | ASN  |
| 10  | K     | 158 | ILE  |
| 11  | L     | 148 | ILE  |
| 26  | a     | 104 | ARG  |
| 4   | E     | 246 | PHE  |

### 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.

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2   | C     | 174/244 (71%)  | 174 (100%) | 0        | 100         | 100 |
| 3   | D     | 196/231 (85%)  | 196 (100%) | 0        | 100         | 100 |
| 4   | E     | 186/187 (100%) | 186 (100%) | 0        | 100         | 100 |
| 5   | F     | 190/202 (94%)  | 190 (100%) | 0        | 100         | 100 |
| 6   | G     | 225/225 (100%) | 225 (100%) | 0        | 100         | 100 |
| 7   | H     | 161/170 (95%)  | 161 (100%) | 0        | 100         | 100 |
| 8   | I     | 207/218 (95%)  | 207 (100%) | 0        | 100         | 100 |
| 9   | J     | 170/174 (98%)  | 170 (100%) | 0        | 100         | 100 |
| 10  | K     | 177/180 (98%)  | 177 (100%) | 0        | 100         | 100 |
| 11  | L     | 157/168 (94%)  | 157 (100%) | 0        | 100         | 100 |
| 12  | M     | 89/173 (51%)   | 89 (100%)  | 0        | 100         | 100 |
| 13  | N     | 142/142 (100%) | 142 (100%) | 0        | 100         | 100 |
| 14  | O     | 104/108 (96%)  | 104 (100%) | 0        | 100         | 100 |
| 15  | P     | 130/131 (99%)  | 130 (100%) | 0        | 100         | 100 |
| 16  | Q     | 106/130 (82%)  | 106 (100%) | 0        | 100         | 100 |
| 17  | R     | 121/130 (93%)  | 120 (99%)  | 1 (1%)   | 73          | 77  |
| 18  | S     | 117/121 (97%)  | 117 (100%) | 0        | 100         | 100 |
| 19  | T     | 114/121 (94%)  | 114 (100%) | 0        | 100         | 100 |
| 20  | U     | 122/132 (92%)  | 122 (100%) | 0        | 100         | 100 |
| 21  | V     | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 22  | W     | 94/107 (88%)   | 94 (100%)  | 0        | 100         | 100 |
| 23  | X     | 67/68 (98%)    | 67 (100%)  | 0        | 100         | 100 |
| 24  | Y     | 112/113 (99%)  | 112 (100%) | 0        | 100         | 100 |
| 25  | Z     | 114/115 (99%)  | 114 (100%) | 0        | 100         | 100 |
| 26  | a     | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 27  | b     | 87/99 (88%)    | 87 (100%)  | 0        | 100         | 100 |
| 28  | c     | 76/76 (100%)   | 76 (100%)  | 0        | 100         | 100 |
| 29  | d     | 57/57 (100%)   | 57 (100%)  | 0        | 100         | 100 |
| 30  | e     | 47/49 (96%)    | 47 (100%)  | 0        | 100         | 100 |
| 31  | f     | 64/140 (46%)   | 64 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 32  | g     | 272/275 (99%)   | 272 (100%)  | 0        | 100         | 100 |
| 33  | h     | 66/103 (64%)    | 66 (100%)   | 0        | 100         | 100 |
| 34  | i     | 49/49 (100%)    | 49 (100%)   | 0        | 100         | 100 |
| 35  | l     | 24/24 (100%)    | 24 (100%)   | 0        | 100         | 100 |
| All | All   | 4238/4683 (90%) | 4237 (100%) | 1 (0%)   | 100         | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | R     | 104 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 50  | ASN  |
| 2   | C     | 70  | ASN  |
| 2   | C     | 132 | GLN  |
| 2   | C     | 141 | ASN  |
| 3   | D     | 53  | GLN  |
| 3   | D     | 75  | GLN  |
| 3   | D     | 159 | GLN  |
| 3   | D     | 163 | GLN  |
| 3   | D     | 179 | ASN  |
| 3   | D     | 186 | ASN  |
| 6   | G     | 17  | HIS  |
| 6   | G     | 112 | HIS  |
| 6   | G     | 197 | ASN  |
| 6   | G     | 216 | ASN  |
| 7   | H     | 79  | HIS  |
| 7   | H     | 82  | ASN  |
| 8   | I     | 110 | ASN  |
| 9   | J     | 168 | HIS  |
| 9   | J     | 186 | ASN  |
| 10  | K     | 64  | ASN  |
| 11  | L     | 113 | GLN  |
| 11  | L     | 124 | HIS  |
| 11  | L     | 132 | GLN  |
| 11  | L     | 134 | HIS  |
| 11  | L     | 154 | GLN  |
| 12  | M     | 7   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | N     | 5   | GLN  |
| 13  | N     | 83  | GLN  |
| 13  | N     | 94  | HIS  |
| 13  | N     | 121 | GLN  |
| 13  | N     | 156 | GLN  |
| 14  | O     | 73  | GLN  |
| 15  | P     | 5   | HIS  |
| 15  | P     | 105 | ASN  |
| 16  | Q     | 20  | GLN  |
| 17  | R     | 35  | GLN  |
| 20  | U     | 19  | ASN  |
| 21  | V     | 137 | GLN  |
| 25  | Z     | 26  | GLN  |
| 25  | Z     | 31  | HIS  |
| 26  | a     | 15  | ASN  |
| 26  | a     | 29  | HIS  |
| 26  | a     | 112 | ASN  |
| 30  | e     | 26  | ASN  |
| 31  | f     | 91  | ASN  |
| 31  | f     | 93  | HIS  |
| 31  | f     | 135 | HIS  |
| 32  | g     | 133 | ASN  |
| 32  | g     | 305 | ASN  |
| 33  | h     | 106 | GLN  |
| 34  | i     | 111 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 2     | 1733/1863 (93%) | 383 (22%)         | 7 (0%)          |
| 36  | y     | 74/75 (98%)     | 33 (44%)          | 0               |
| 37  | z     | 91/93 (97%)     | 31 (34%)          | 0               |
| All | All   | 1898/2031 (93%) | 447 (23%)         | 7 (0%)          |

All (447) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 2   | A    |
| 1   | 2     | 4   | C    |
| 1   | 2     | 26  | U    |
| 1   | 2     | 33  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 39  | A    |
| 1   | 2     | 41  | G    |
| 1   | 2     | 42  | A    |
| 1   | 2     | 44  | U    |
| 1   | 2     | 46  | A    |
| 1   | 2     | 49  | C    |
| 1   | 2     | 55  | U    |
| 1   | 2     | 56  | G    |
| 1   | 2     | 60  | A    |
| 1   | 2     | 65  | C    |
| 1   | 2     | 67  | C    |
| 1   | 2     | 68  | A    |
| 1   | 2     | 72  | C    |
| 1   | 2     | 73  | C    |
| 1   | 2     | 74  | G    |
| 1   | 2     | 76  | U    |
| 1   | 2     | 79  | A    |
| 1   | 2     | 80  | G    |
| 1   | 2     | 93  | U    |
| 1   | 2     | 94  | G    |
| 1   | 2     | 99  | A    |
| 1   | 2     | 101 | U    |
| 1   | 2     | 110 | U    |
| 1   | 2     | 113 | G    |
| 1   | 2     | 114 | G    |
| 1   | 2     | 115 | U    |
| 1   | 2     | 126 | G    |
| 1   | 2     | 127 | C    |
| 1   | 2     | 140 | U    |
| 1   | 2     | 143 | U    |
| 1   | 2     | 147 | A    |
| 1   | 2     | 148 | U    |
| 1   | 2     | 153 | G    |
| 1   | 2     | 161 | U    |
| 1   | 2     | 168 | C    |
| 1   | 2     | 169 | U    |
| 1   | 2     | 170 | A    |
| 1   | 2     | 171 | A    |
| 1   | 2     | 172 | U    |
| 1   | 2     | 173 | A    |
| 1   | 2     | 178 | C    |
| 1   | 2     | 179 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 181 | A    |
| 1   | 2     | 182 | C    |
| 1   | 2     | 183 | G    |
| 1   | 2     | 191 | C    |
| 1   | 2     | 197 | U    |
| 1   | 2     | 202 | U    |
| 1   | 2     | 204 | G    |
| 1   | 2     | 206 | A    |
| 1   | 2     | 223 | A    |
| 1   | 2     | 224 | U    |
| 1   | 2     | 225 | C    |
| 1   | 2     | 226 | A    |
| 1   | 2     | 239 | U    |
| 1   | 2     | 271 | G    |
| 1   | 2     | 276 | U    |
| 1   | 2     | 277 | U    |
| 1   | 2     | 278 | U    |
| 1   | 2     | 285 | U    |
| 1   | 2     | 293 | A    |
| 1   | 2     | 296 | U    |
| 1   | 2     | 297 | C    |
| 1   | 2     | 298 | G    |
| 1   | 2     | 299 | G    |
| 1   | 2     | 300 | G    |
| 1   | 2     | 305 | U    |
| 1   | 2     | 308 | C    |
| 1   | 2     | 309 | A    |
| 1   | 2     | 311 | C    |
| 1   | 2     | 315 | C    |
| 1   | 2     | 316 | C    |
| 1   | 2     | 317 | G    |
| 1   | 2     | 322 | G    |
| 1   | 2     | 325 | G    |
| 1   | 2     | 337 | G    |
| 1   | 2     | 340 | C    |
| 1   | 2     | 343 | C    |
| 1   | 2     | 347 | C    |
| 1   | 2     | 350 | A    |
| 1   | 2     | 352 | C    |
| 1   | 2     | 354 | A    |
| 1   | 2     | 358 | U    |
| 1   | 2     | 359 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 365 | U    |
| 1   | 2     | 375 | G    |
| 1   | 2     | 376 | C    |
| 1   | 2     | 388 | A    |
| 1   | 2     | 390 | C    |
| 1   | 2     | 399 | C    |
| 1   | 2     | 403 | G    |
| 1   | 2     | 416 | A    |
| 1   | 2     | 418 | U    |
| 1   | 2     | 438 | A    |
| 1   | 2     | 440 | C    |
| 1   | 2     | 442 | G    |
| 1   | 2     | 457 | G    |
| 1   | 2     | 462 | C    |
| 1   | 2     | 466 | A    |
| 1   | 2     | 475 | A    |
| 1   | 2     | 477 | U    |
| 1   | 2     | 481 | C    |
| 1   | 2     | 483 | A    |
| 1   | 2     | 487 | C    |
| 1   | 2     | 491 | C    |
| 1   | 2     | 492 | C    |
| 1   | 2     | 506 | A    |
| 1   | 2     | 507 | C    |
| 1   | 2     | 513 | A    |
| 1   | 2     | 514 | U    |
| 1   | 2     | 515 | A    |
| 1   | 2     | 517 | C    |
| 1   | 2     | 518 | A    |
| 1   | 2     | 541 | U    |
| 1   | 2     | 542 | G    |
| 1   | 2     | 547 | U    |
| 1   | 2     | 548 | G    |
| 1   | 2     | 553 | G    |
| 1   | 2     | 554 | A    |
| 1   | 2     | 563 | U    |
| 1   | 2     | 566 | A    |
| 1   | 2     | 577 | A    |
| 1   | 2     | 579 | G    |
| 1   | 2     | 580 | A    |
| 1   | 2     | 581 | U    |
| 1   | 2     | 583 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 596 | G    |
| 1   | 2     | 597 | U    |
| 1   | 2     | 598 | C    |
| 1   | 2     | 604 | G    |
| 1   | 2     | 607 | G    |
| 1   | 2     | 613 | G    |
| 1   | 2     | 617 | U    |
| 1   | 2     | 621 | U    |
| 1   | 2     | 633 | A    |
| 1   | 2     | 640 | A    |
| 1   | 2     | 645 | A    |
| 1   | 2     | 648 | U    |
| 1   | 2     | 649 | G    |
| 1   | 2     | 650 | C    |
| 1   | 2     | 658 | A    |
| 1   | 2     | 659 | A    |
| 1   | 2     | 661 | A    |
| 1   | 2     | 662 | A    |
| 1   | 2     | 663 | G    |
| 1   | 2     | 674 | G    |
| 1   | 2     | 678 | U    |
| 1   | 2     | 679 | U    |
| 1   | 2     | 680 | G    |
| 1   | 2     | 682 | G    |
| 1   | 2     | 729 | C    |
| 1   | 2     | 735 | C    |
| 1   | 2     | 736 | C    |
| 1   | 2     | 737 | C    |
| 1   | 2     | 738 | U    |
| 1   | 2     | 739 | U    |
| 1   | 2     | 740 | G    |
| 1   | 2     | 741 | C    |
| 1   | 2     | 742 | C    |
| 1   | 2     | 743 | U    |
| 1   | 2     | 744 | C    |
| 1   | 2     | 747 | G    |
| 1   | 2     | 748 | G    |
| 1   | 2     | 749 | C    |
| 1   | 2     | 750 | G    |
| 1   | 2     | 789 | G    |
| 1   | 2     | 794 | G    |
| 1   | 2     | 796 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 800 | U    |
| 1   | 2     | 807 | A    |
| 1   | 2     | 818 | U    |
| 1   | 2     | 819 | U    |
| 1   | 2     | 820 | C    |
| 1   | 2     | 823 | A    |
| 1   | 2     | 827 | G    |
| 1   | 2     | 832 | G    |
| 1   | 2     | 833 | A    |
| 1   | 2     | 835 | C    |
| 1   | 2     | 837 | G    |
| 1   | 2     | 843 | A    |
| 1   | 2     | 868 | A    |
| 1   | 2     | 869 | G    |
| 1   | 2     | 870 | G    |
| 1   | 2     | 873 | C    |
| 1   | 2     | 874 | G    |
| 1   | 2     | 883 | U    |
| 1   | 2     | 886 | U    |
| 1   | 2     | 894 | U    |
| 1   | 2     | 901 | C    |
| 1   | 2     | 903 | G    |
| 1   | 2     | 907 | C    |
| 1   | 2     | 909 | A    |
| 1   | 2     | 910 | U    |
| 1   | 2     | 913 | U    |
| 1   | 2     | 915 | A    |
| 1   | 2     | 916 | A    |
| 1   | 2     | 918 | A    |
| 1   | 2     | 929 | G    |
| 1   | 2     | 930 | G    |
| 1   | 2     | 951 | A    |
| 1   | 2     | 952 | G    |
| 1   | 2     | 956 | U    |
| 1   | 2     | 957 | G    |
| 1   | 2     | 966 | G    |
| 1   | 2     | 967 | G    |
| 1   | 2     | 980 | C    |
| 1   | 2     | 981 | G    |
| 1   | 2     | 986 | A    |
| 1   | 2     | 988 | A    |
| 1   | 2     | 995 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1004 | A    |
| 1   | 2     | 1012 | U    |
| 1   | 2     | 1013 | U    |
| 1   | 2     | 1016 | A    |
| 1   | 2     | 1019 | A    |
| 1   | 2     | 1022 | C    |
| 1   | 2     | 1023 | A    |
| 1   | 2     | 1041 | U    |
| 1   | 2     | 1045 | A    |
| 1   | 2     | 1049 | C    |
| 1   | 2     | 1051 | A    |
| 1   | 2     | 1056 | A    |
| 1   | 2     | 1057 | U    |
| 1   | 2     | 1058 | A    |
| 1   | 2     | 1076 | A    |
| 1   | 2     | 1079 | A    |
| 1   | 2     | 1081 | C    |
| 1   | 2     | 1095 | G    |
| 1   | 2     | 1107 | U    |
| 1   | 2     | 1108 | U    |
| 1   | 2     | 1112 | C    |
| 1   | 2     | 1113 | C    |
| 1   | 2     | 1125 | G    |
| 1   | 2     | 1129 | A    |
| 1   | 2     | 1135 | C    |
| 1   | 2     | 1144 | A    |
| 1   | 2     | 1145 | A    |
| 1   | 2     | 1146 | A    |
| 1   | 2     | 1150 | U    |
| 1   | 2     | 1151 | U    |
| 1   | 2     | 1153 | G    |
| 1   | 2     | 1160 | G    |
| 1   | 2     | 1164 | G    |
| 1   | 2     | 1190 | A    |
| 1   | 2     | 1191 | A    |
| 1   | 2     | 1192 | A    |
| 1   | 2     | 1203 | G    |
| 1   | 2     | 1204 | A    |
| 1   | 2     | 1211 | C    |
| 1   | 2     | 1212 | C    |
| 1   | 2     | 1217 | G    |
| 1   | 2     | 1220 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1238 | U    |
| 1   | 2     | 1244 | U    |
| 1   | 2     | 1245 | C    |
| 1   | 2     | 1247 | A    |
| 1   | 2     | 1249 | A    |
| 1   | 2     | 1252 | G    |
| 1   | 2     | 1253 | G    |
| 1   | 2     | 1254 | A    |
| 1   | 2     | 1261 | A    |
| 1   | 2     | 1266 | G    |
| 1   | 2     | 1269 | C    |
| 1   | 2     | 1271 | G    |
| 1   | 2     | 1280 | A    |
| 1   | 2     | 1285 | U    |
| 1   | 2     | 1297 | A    |
| 1   | 2     | 1298 | G    |
| 1   | 2     | 1299 | C    |
| 1   | 2     | 1304 | U    |
| 1   | 2     | 1317 | G    |
| 1   | 2     | 1323 | G    |
| 1   | 2     | 1333 | C    |
| 1   | 2     | 1339 | U    |
| 1   | 2     | 1352 | G    |
| 1   | 2     | 1354 | U    |
| 1   | 2     | 1359 | C    |
| 1   | 2     | 1360 | U    |
| 1   | 2     | 1365 | A    |
| 1   | 2     | 1367 | U    |
| 1   | 2     | 1368 | U    |
| 1   | 2     | 1374 | A    |
| 1   | 2     | 1386 | U    |
| 1   | 2     | 1399 | C    |
| 1   | 2     | 1408 | C    |
| 1   | 2     | 1409 | G    |
| 1   | 2     | 1411 | C    |
| 1   | 2     | 1414 | C    |
| 1   | 2     | 1415 | C    |
| 1   | 2     | 1420 | G    |
| 1   | 2     | 1427 | G    |
| 1   | 2     | 1431 | C    |
| 1   | 2     | 1432 | C    |
| 1   | 2     | 1433 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1438 | U    |
| 1   | 2     | 1440 | U    |
| 1   | 2     | 1445 | G    |
| 1   | 2     | 1446 | G    |
| 1   | 2     | 1448 | A    |
| 1   | 2     | 1449 | C    |
| 1   | 2     | 1450 | A    |
| 1   | 2     | 1459 | U    |
| 1   | 2     | 1471 | G    |
| 1   | 2     | 1472 | A    |
| 1   | 2     | 1473 | U    |
| 1   | 2     | 1485 | A    |
| 1   | 2     | 1486 | G    |
| 1   | 2     | 1489 | C    |
| 1   | 2     | 1490 | U    |
| 1   | 2     | 1491 | G    |
| 1   | 2     | 1494 | A    |
| 1   | 2     | 1503 | G    |
| 1   | 2     | 1506 | G    |
| 1   | 2     | 1507 | U    |
| 1   | 2     | 1508 | C    |
| 1   | 2     | 1514 | U    |
| 1   | 2     | 1516 | C    |
| 1   | 2     | 1517 | A    |
| 1   | 2     | 1528 | A    |
| 1   | 2     | 1531 | G    |
| 1   | 2     | 1535 | G    |
| 1   | 2     | 1539 | C    |
| 1   | 2     | 1543 | G    |
| 1   | 2     | 1547 | G    |
| 1   | 2     | 1548 | C    |
| 1   | 2     | 1549 | C    |
| 1   | 2     | 1550 | U    |
| 1   | 2     | 1551 | A    |
| 1   | 2     | 1555 | U    |
| 1   | 2     | 1565 | G    |
| 1   | 2     | 1569 | C    |
| 1   | 2     | 1574 | A    |
| 1   | 2     | 1575 | A    |
| 1   | 2     | 1580 | U    |
| 1   | 2     | 1582 | G    |
| 1   | 2     | 1583 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1593 | G    |
| 1   | 2     | 1596 | A    |
| 1   | 2     | 1601 | G    |
| 1   | 2     | 1616 | U    |
| 1   | 2     | 1617 | U    |
| 1   | 2     | 1618 | A    |
| 1   | 2     | 1641 | C    |
| 1   | 2     | 1643 | G    |
| 1   | 2     | 1649 | G    |
| 1   | 2     | 1656 | A    |
| 1   | 2     | 1659 | A    |
| 1   | 2     | 1660 | G    |
| 1   | 2     | 1675 | G    |
| 1   | 2     | 1694 | A    |
| 1   | 2     | 1695 | C    |
| 1   | 2     | 1696 | C    |
| 1   | 2     | 1715 | U    |
| 1   | 2     | 1716 | U    |
| 1   | 2     | 1717 | G    |
| 1   | 2     | 1724 | U    |
| 1   | 2     | 1732 | G    |
| 1   | 2     | 1739 | G    |
| 1   | 2     | 1777 | C    |
| 1   | 2     | 1778 | G    |
| 1   | 2     | 1791 | U    |
| 1   | 2     | 1792 | C    |
| 1   | 2     | 1814 | G    |
| 1   | 2     | 1817 | A    |
| 1   | 2     | 1823 | G    |
| 1   | 2     | 1825 | A    |
| 1   | 2     | 1832 | U    |
| 1   | 2     | 1833 | U    |
| 1   | 2     | 1834 | U    |
| 1   | 2     | 1843 | G    |
| 1   | 2     | 1846 | C    |
| 1   | 2     | 1853 | A    |
| 1   | 2     | 1855 | G    |
| 1   | 2     | 1856 | G    |
| 1   | 2     | 1857 | A    |
| 1   | 2     | 1858 | U    |
| 1   | 2     | 1859 | C    |
| 1   | 2     | 1861 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1862 | U    |
| 36  | y     | 2    | G    |
| 36  | y     | 4    | A    |
| 36  | y     | 6    | A    |
| 36  | y     | 8    | U    |
| 36  | y     | 9    | G    |
| 36  | y     | 10   | G    |
| 36  | y     | 11   | C    |
| 36  | y     | 12   | G    |
| 36  | y     | 14   | A    |
| 36  | y     | 15   | G    |
| 36  | y     | 17   | G    |
| 36  | y     | 18   | G    |
| 36  | y     | 19   | A    |
| 36  | y     | 20   | A    |
| 36  | y     | 21   | G    |
| 36  | y     | 26   | C    |
| 36  | y     | 32   | C    |
| 36  | y     | 44   | G    |
| 36  | y     | 45   | G    |
| 36  | y     | 46   | U    |
| 36  | y     | 47   | C    |
| 36  | y     | 48   | G    |
| 36  | y     | 52   | G    |
| 36  | y     | 53   | A    |
| 36  | y     | 54   | U    |
| 36  | y     | 55   | C    |
| 36  | y     | 58   | A    |
| 36  | y     | 60   | C    |
| 36  | y     | 62   | A    |
| 36  | y     | 71   | U    |
| 36  | y     | 72   | A    |
| 36  | y     | 73   | C    |
| 36  | y     | 75   | A    |
| 37  | z     | 525  | A    |
| 37  | z     | 531  | C    |
| 37  | z     | 533  | G    |
| 37  | z     | 534  | A    |
| 37  | z     | 535  | A    |
| 37  | z     | 536  | C    |
| 37  | z     | 538  | C    |
| 37  | z     | 539  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | z     | 540 | C    |
| 37  | z     | 546 | G    |
| 37  | z     | 549 | G    |
| 37  | z     | 550 | A    |
| 37  | z     | 556 | G    |
| 37  | z     | 557 | C    |
| 37  | z     | 558 | C    |
| 37  | z     | 562 | G    |
| 37  | z     | 564 | G    |
| 37  | z     | 565 | G    |
| 37  | z     | 568 | A    |
| 37  | z     | 575 | A    |
| 37  | z     | 576 | C    |
| 37  | z     | 577 | G    |
| 37  | z     | 578 | U    |
| 37  | z     | 585 | G    |
| 37  | z     | 586 | A    |
| 37  | z     | 587 | U    |
| 37  | z     | 594 | G    |
| 37  | z     | 832 | A    |
| 37  | z     | 833 | U    |
| 37  | z     | 837 | G    |
| 37  | z     | 838 | C    |

All (7) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 514  | U    |
| 1   | 2     | 516  | A    |
| 1   | 2     | 740  | G    |
| 1   | 2     | 747  | G    |
| 1   | 2     | 914  | U    |
| 1   | 2     | 1338 | U    |
| 1   | 2     | 1431 | C    |

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | 2     | 2                |
| 37  | z     | 1                |
| 8   | I     | 1                |
| 26  | a     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | z     | 601:C     | O3'    | 831:A     | P      | 113.27       |
| 1     | 2     | 730:C     | O3'    | 731:C     | P      | 8.43         |
| 1     | 2     | 363:G     | O3'    | 364:G     | P      | 3.41         |
| 1     | I     | 217:MET   | C      | 218:LYS   | N      | 3.36         |
| 1     | a     | 9:THR     | C      | 10:ARG    | N      | 3.13         |

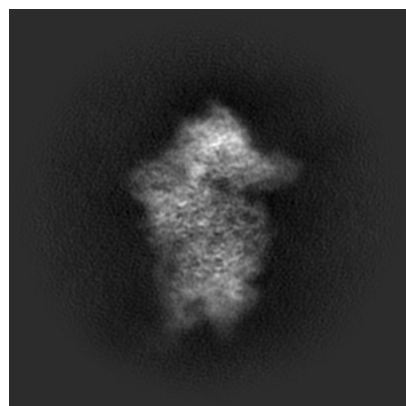
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64644. These allow visual inspection of the internal detail of the map and identification of artifacts.

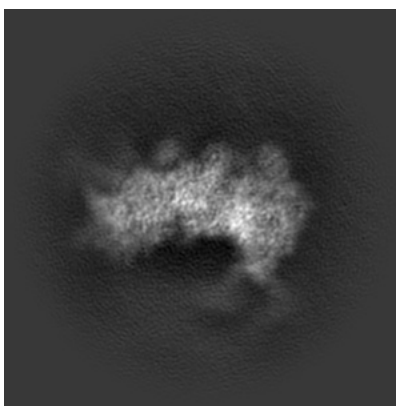
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

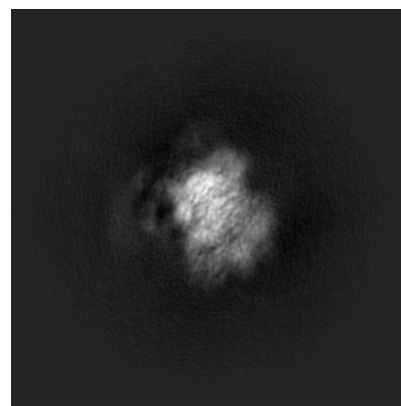
#### 6.1.1 Primary map



X

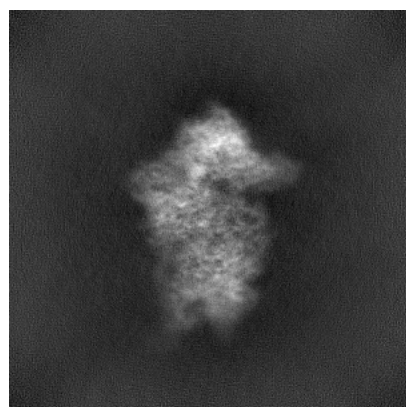


Y

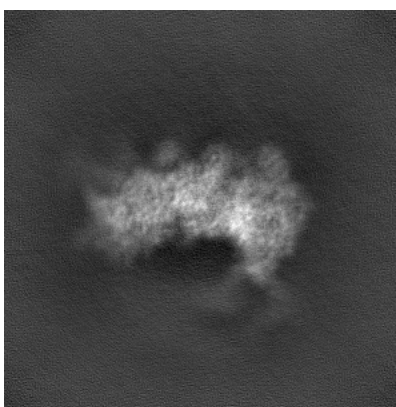


Z

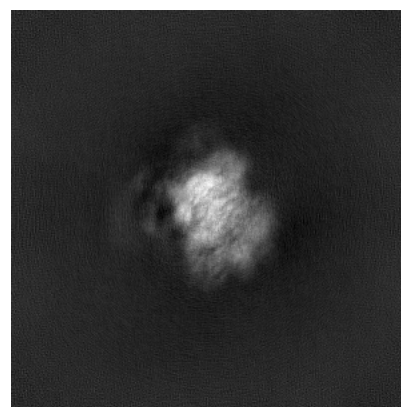
#### 6.1.2 Raw map



X



Y

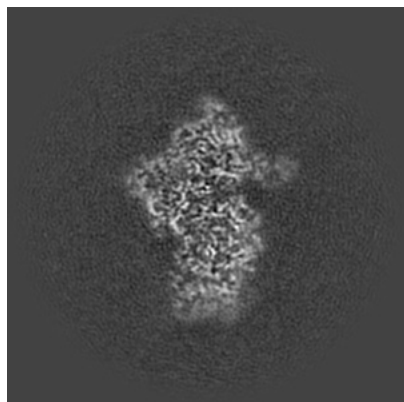


Z

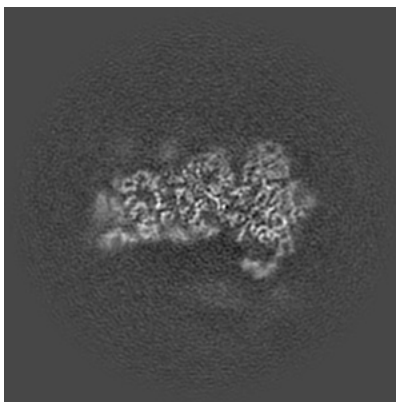
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

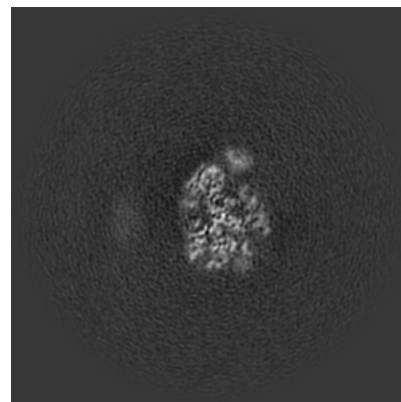
### 6.2.1 Primary map



X Index: 200

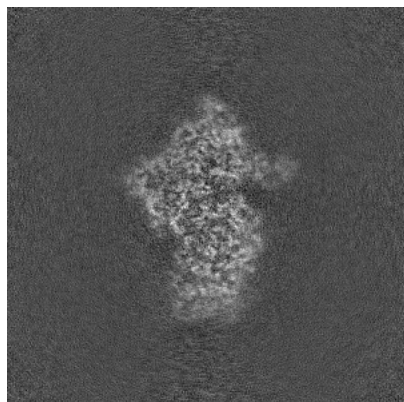


Y Index: 200

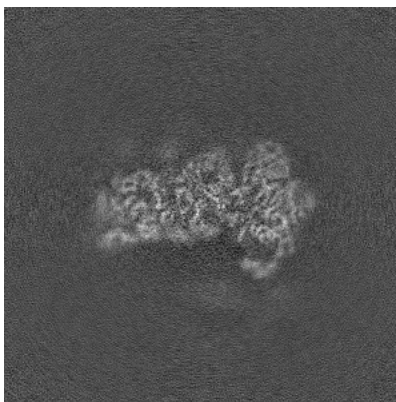


Z Index: 200

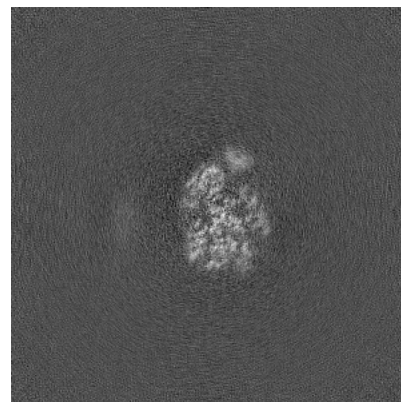
### 6.2.2 Raw map



X Index: 200



Y Index: 200

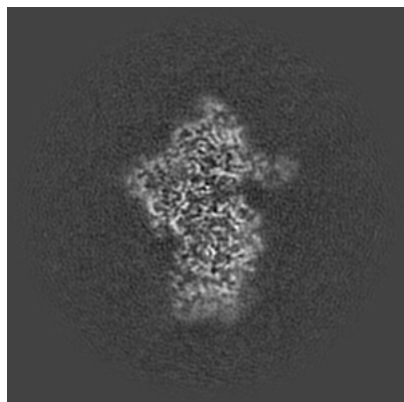


Z Index: 200

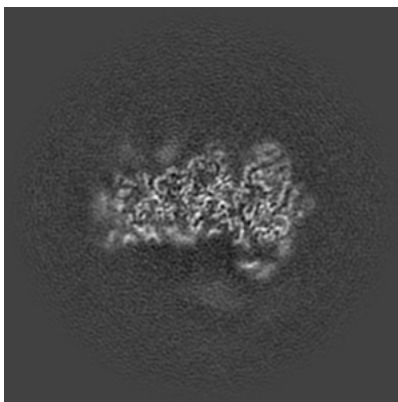
The images above show central slices of the map in three orthogonal directions.

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

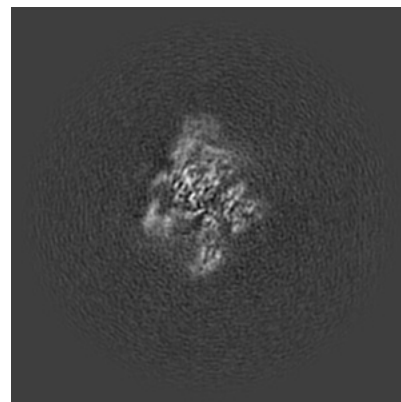
### 6.3.1 Primary map



X Index: 200

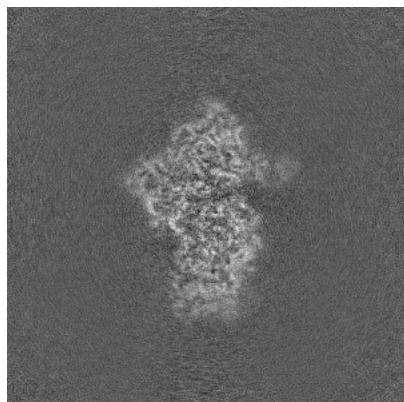


Y Index: 196

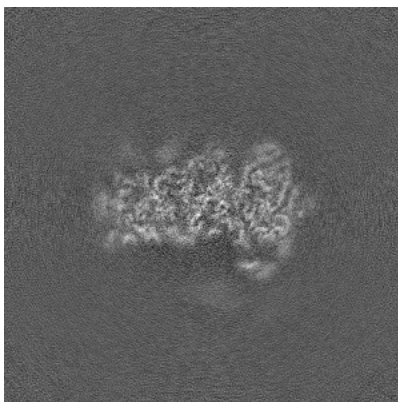


Z Index: 243

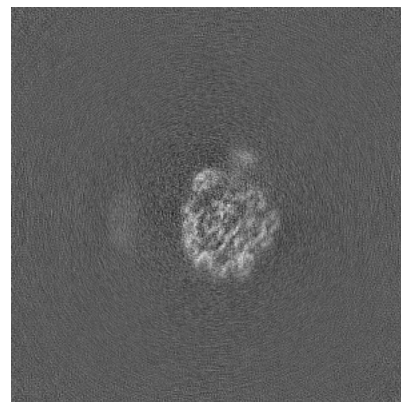
### 6.3.2 Raw map



X Index: 199



Y Index: 196

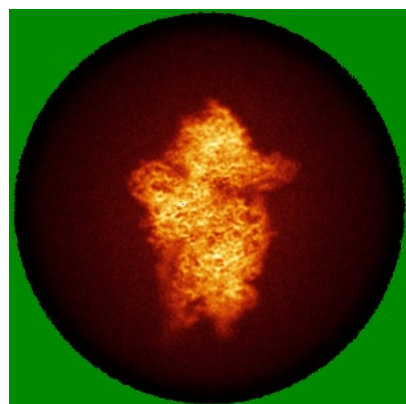


Z Index: 208

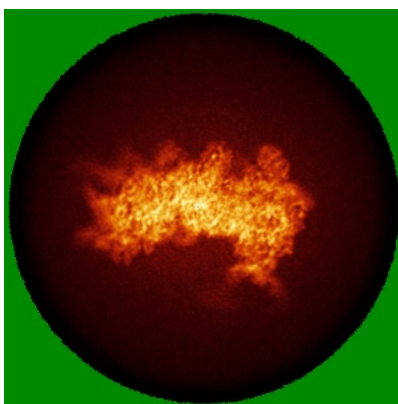
The images above show the largest variance slices of the map in three orthogonal directions.

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

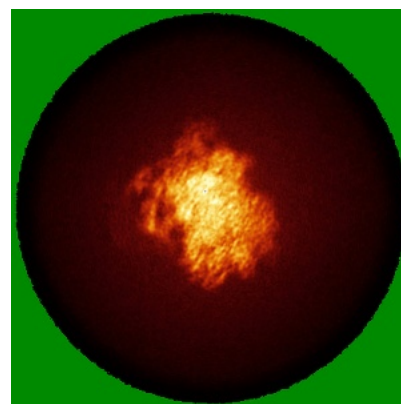
### 6.4.1 Primary map



X

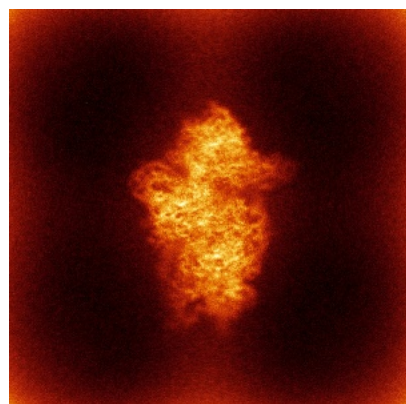


Y

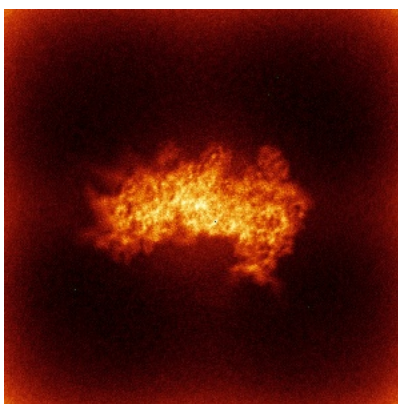


Z

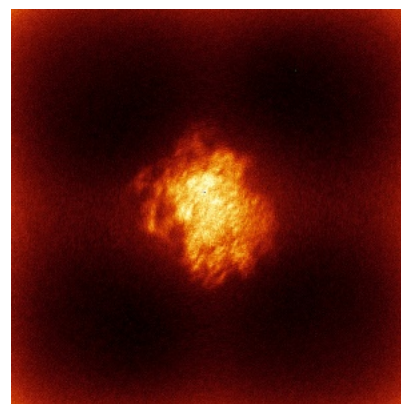
### 6.4.2 Raw map



X



Y

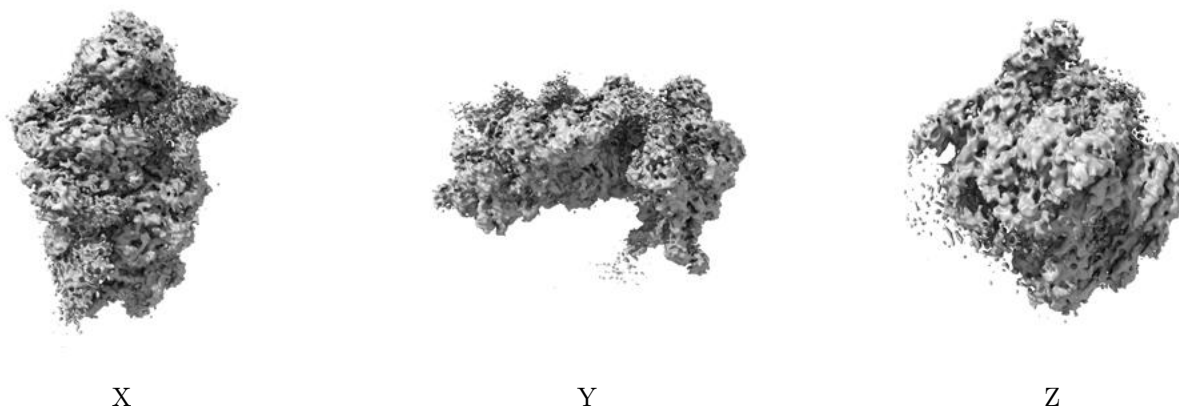


Z

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.

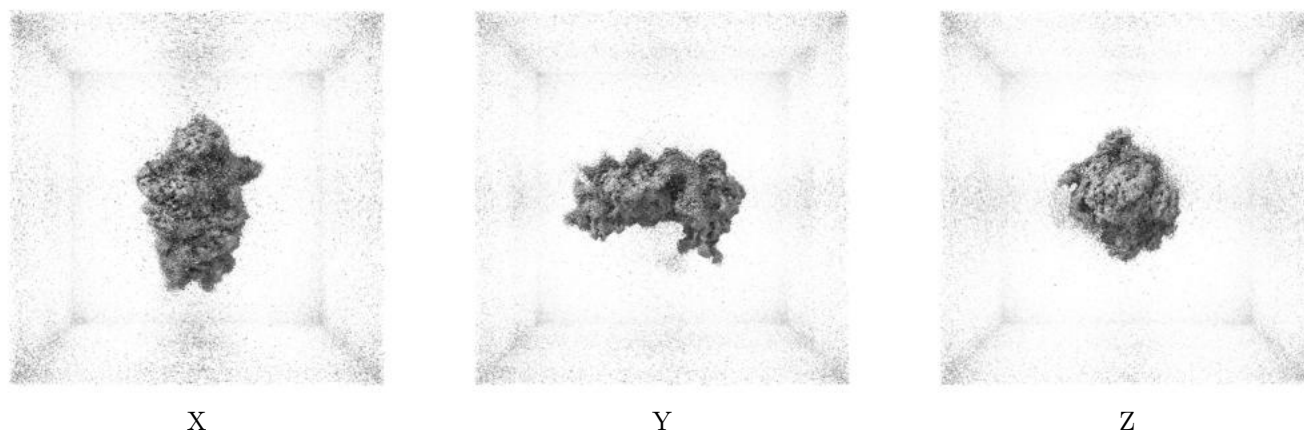
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0811. 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.

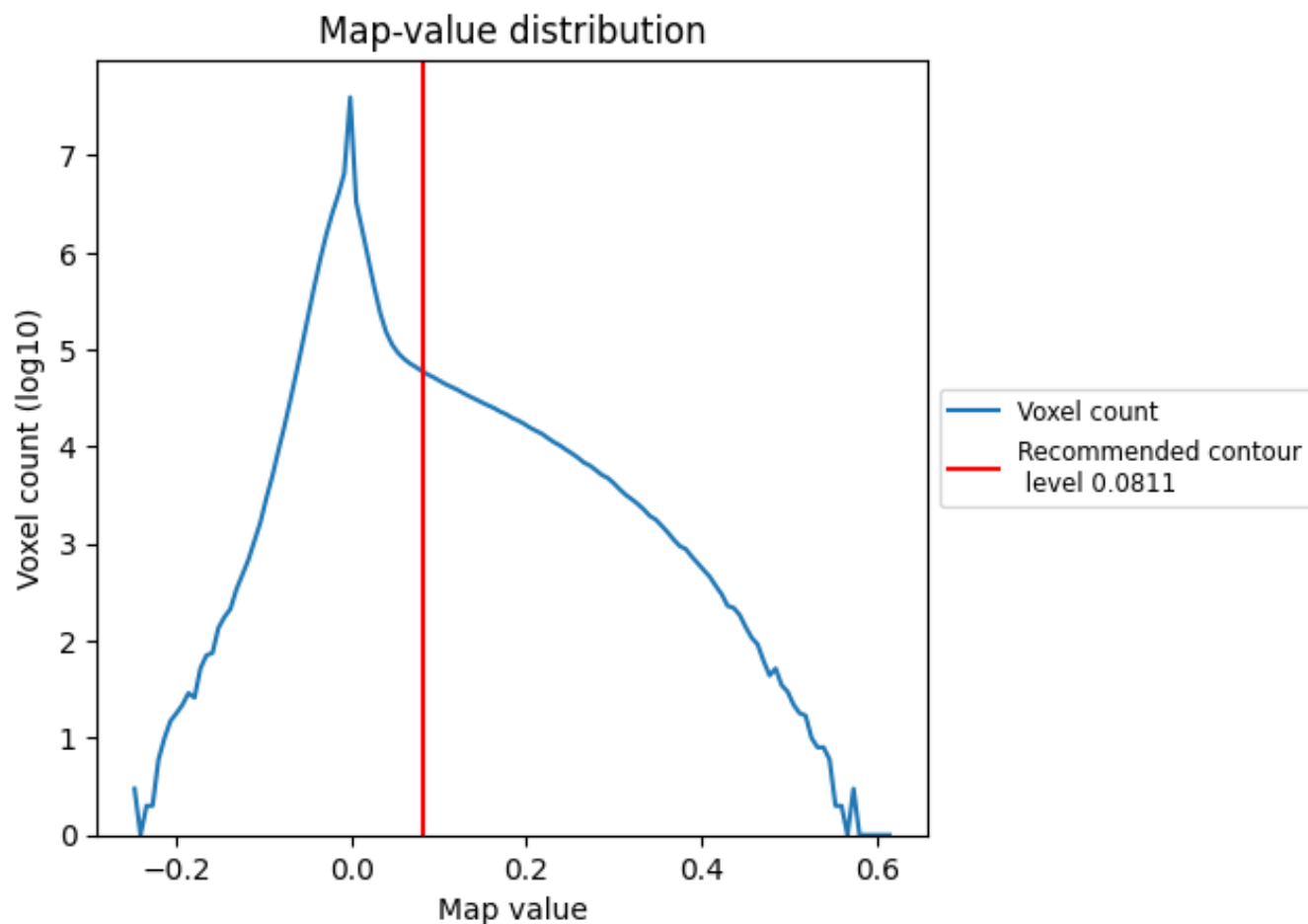
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

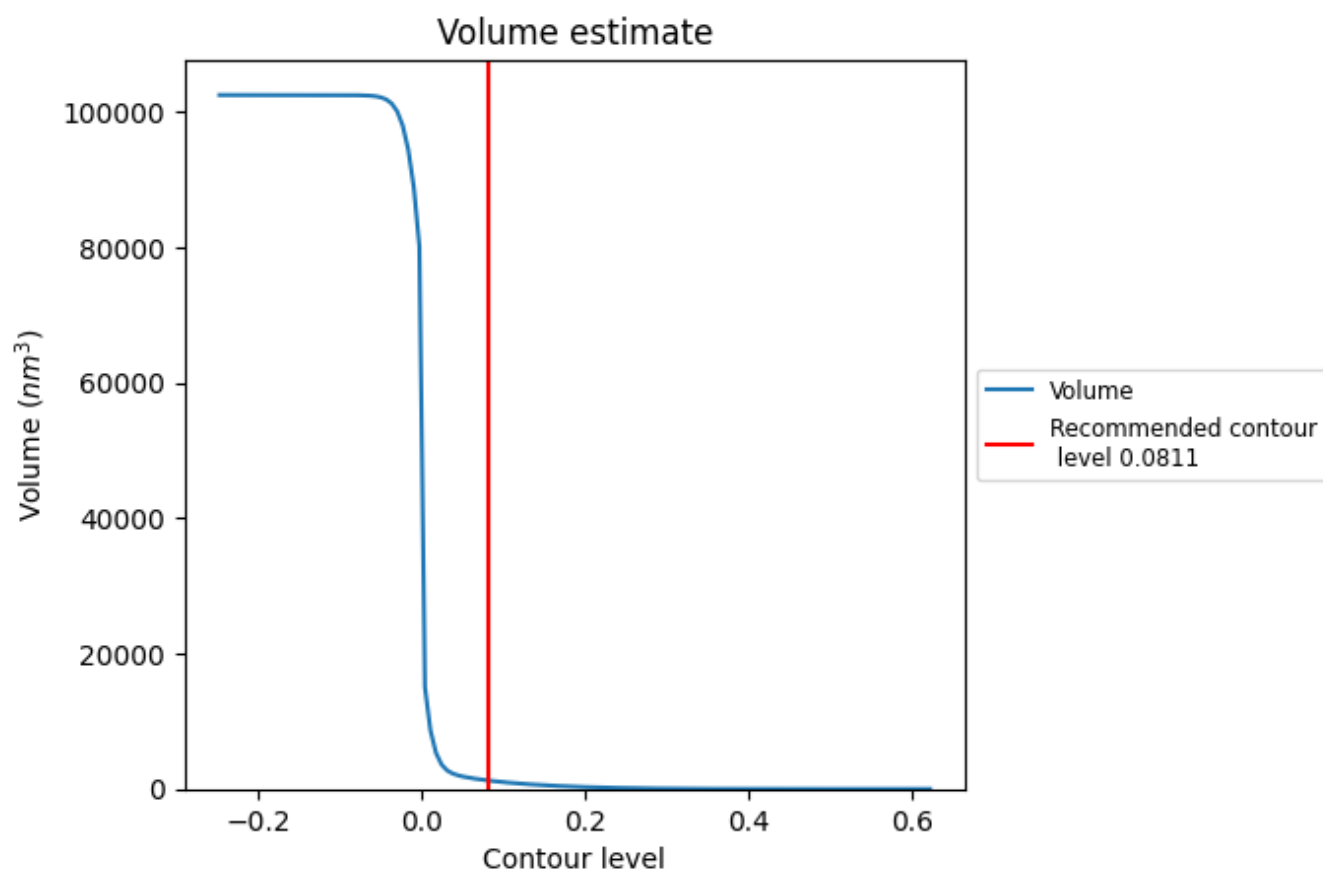
This section contains the results of statistical analysis of the map.

### 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.

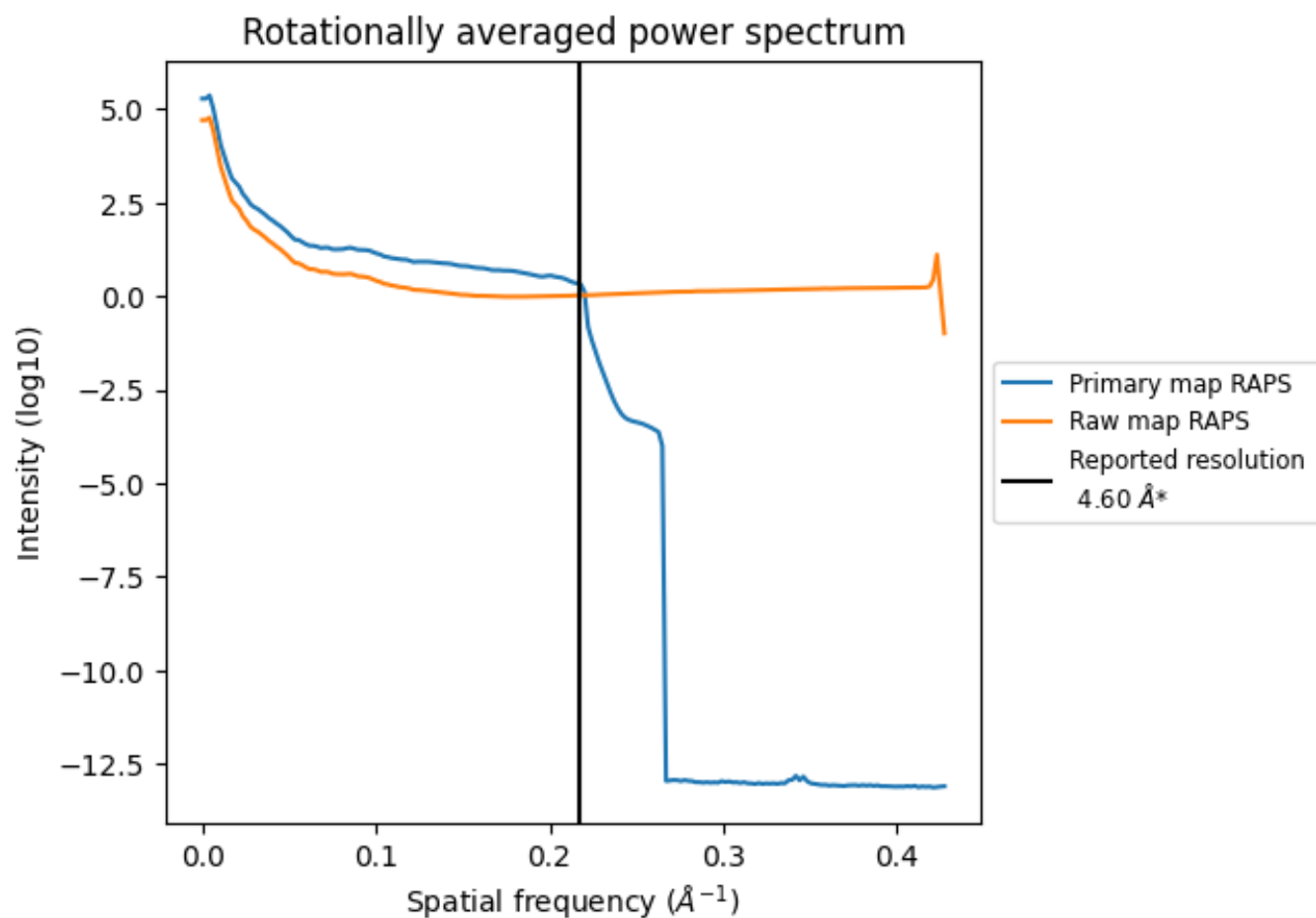
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1251 nm<sup>3</sup>; this corresponds to an approximate mass of 1130 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 ⓘ

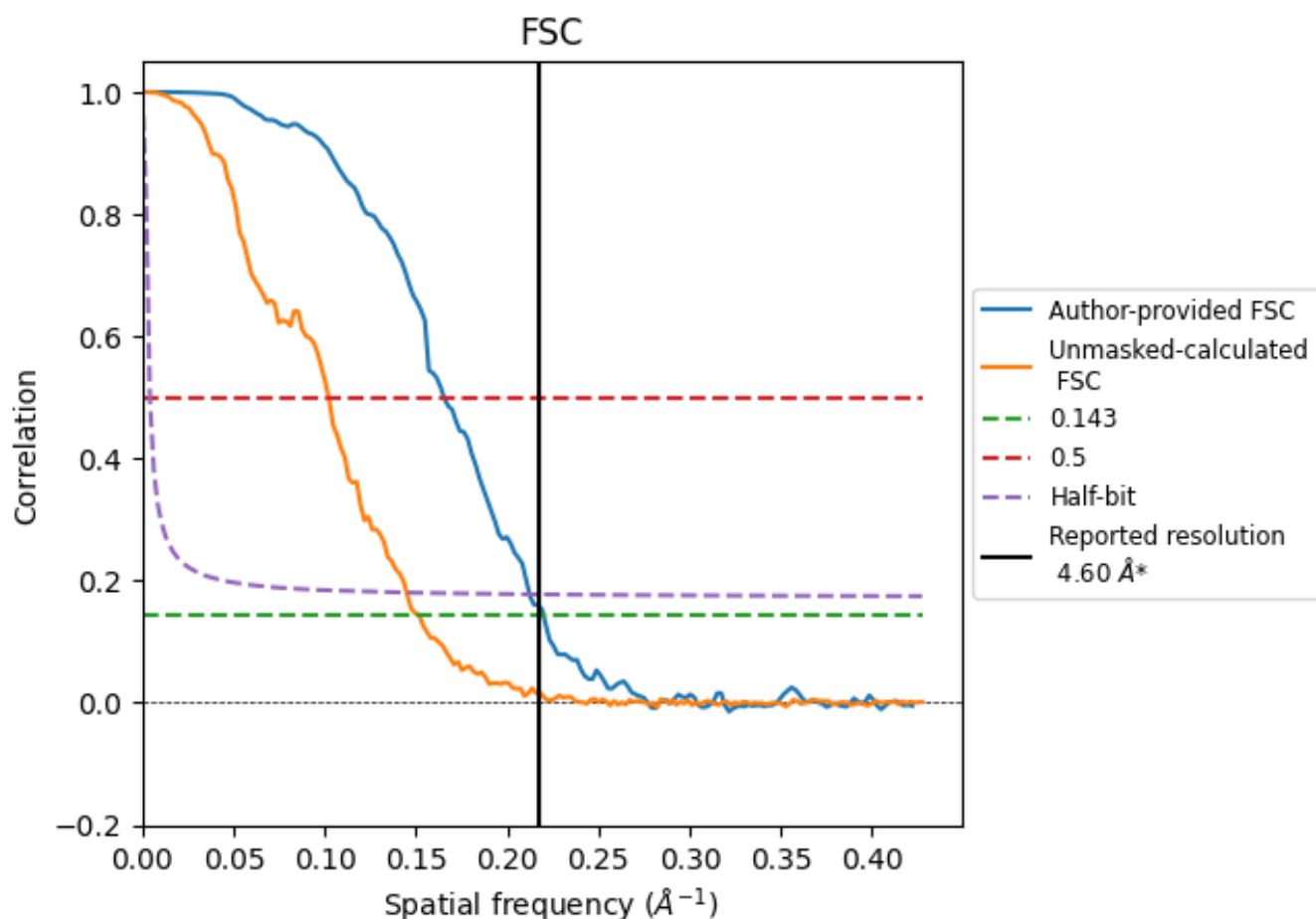


\*Reported resolution corresponds to spatial frequency of 0.217 Å<sup>-1</sup>

## 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  $0.217 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

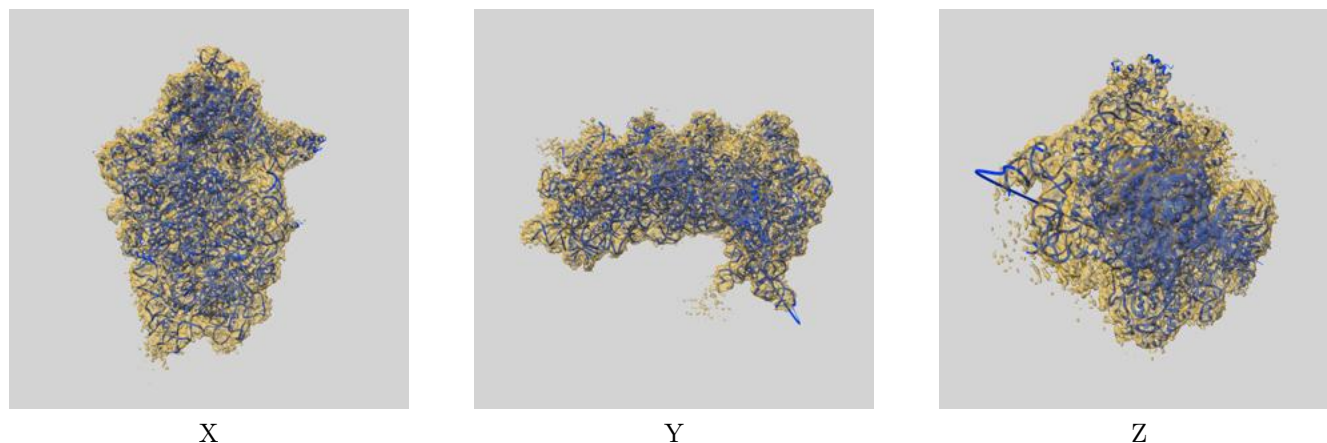
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.60                               | -    | -        |
| Author-provided FSC curve | 4.55                               | 6.05 | 4.71     |
| Unmasked-calculated*      | 6.58                               | 9.79 | 6.90     |

\*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 6.58 differs from the reported value 4.6 by more than 10 %

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

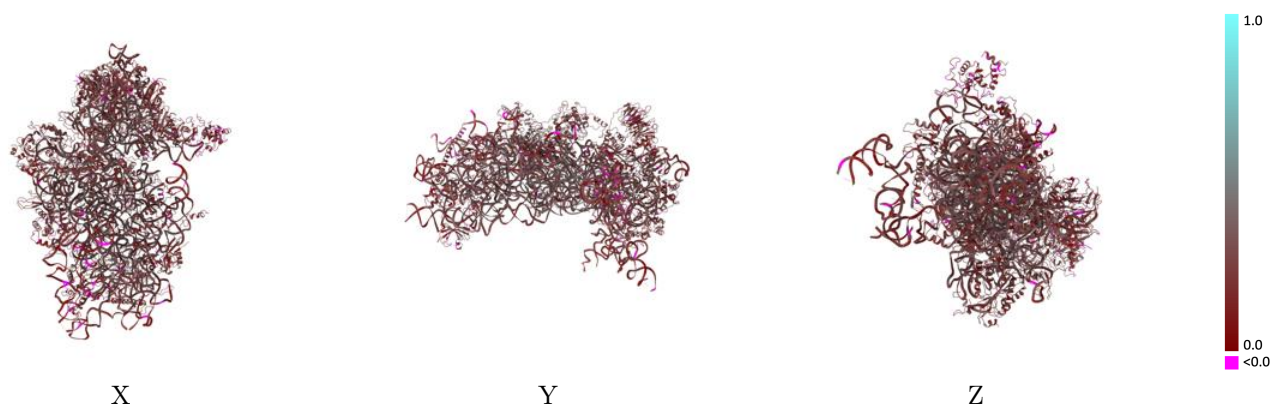
This section contains information regarding the fit between EMDB map EMD-64644 and PDB model 9UZK. Per-residue inclusion information can be found in section 3 on page 11.

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



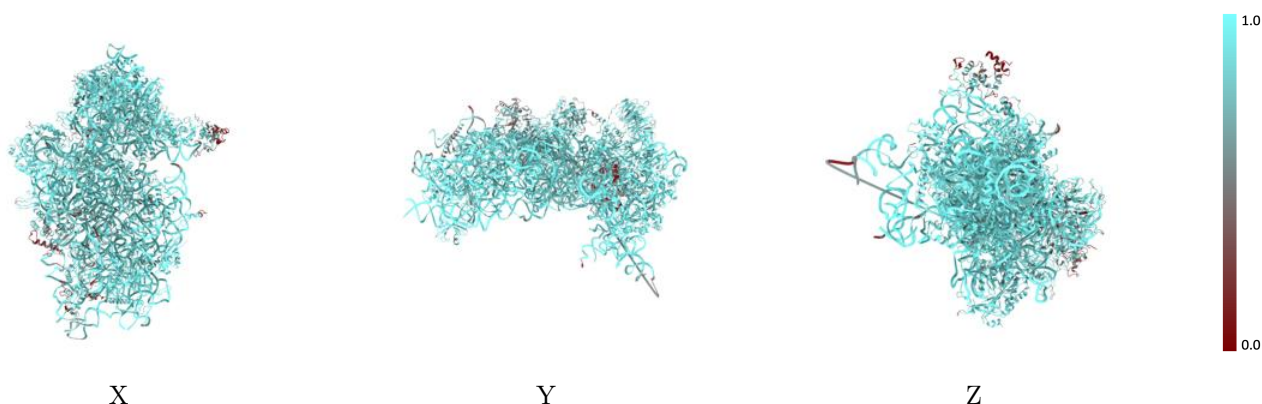
The images above show the 3D surface view of the map at the recommended contour level 0.0811 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



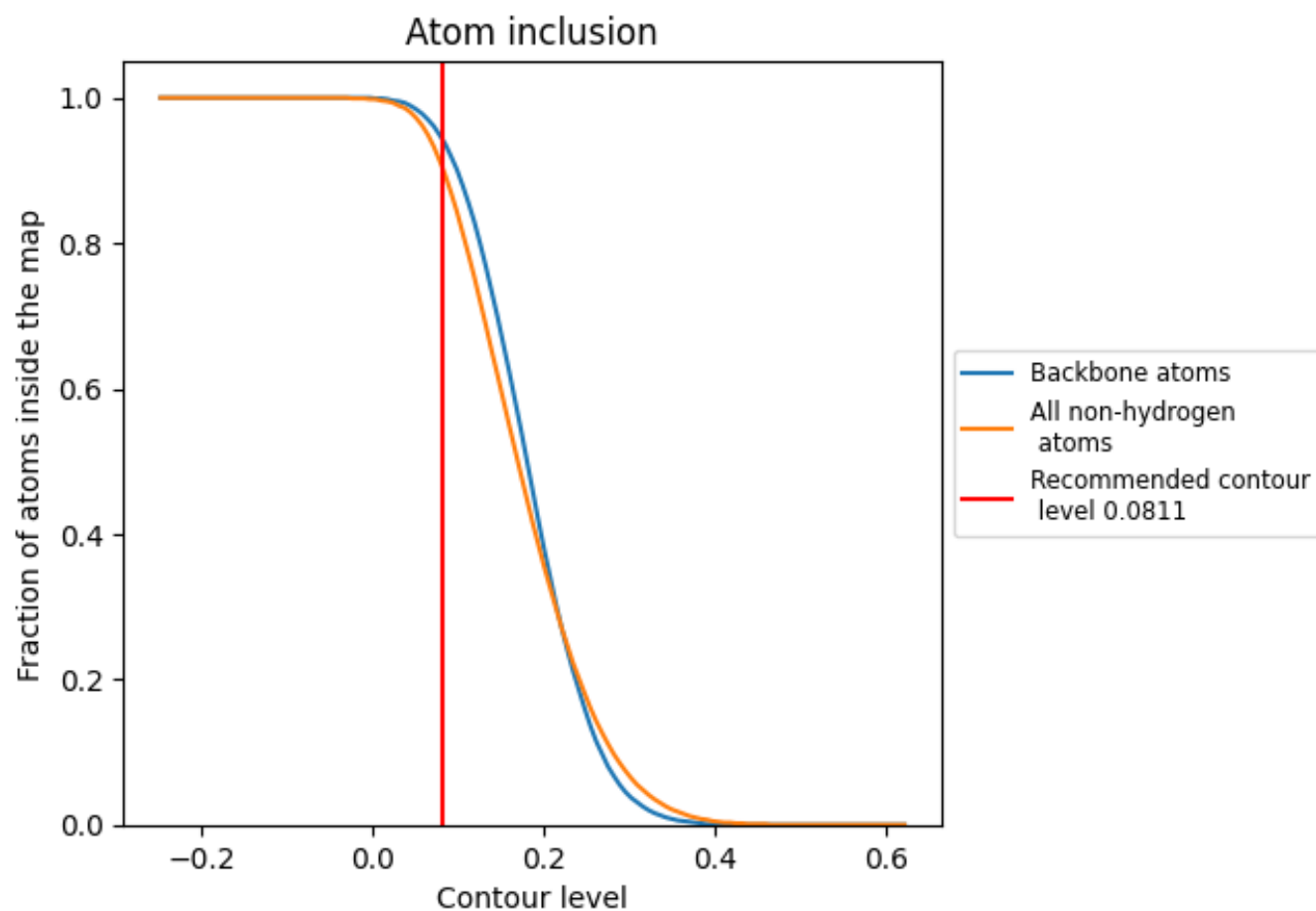
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0811).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.0811) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9060   |  0.2730   |
| 2     |  0.9640   |  0.2880   |
| C     |  0.7970   |  0.2600   |
| D     |  0.8920   |  0.2580   |
| E     |  0.8620   |  0.2970   |
| F     |  0.8480   |  0.2630   |
| G     |  0.9100   |  0.2880   |
| H     |  0.8900   |  0.2790   |
| I     |  0.8790   |  0.2400   |
| J     |  0.5590   |  0.2290   |
| K     |  0.8290   |  0.2540   |
| L     |  0.8730   |  0.2790   |
| M     |  0.8990   |  0.2530   |
| N     |  0.7630   |  0.2890   |
| O     |  0.4810  |  0.1680  |
| P     |  0.8830 |  0.2890 |
| Q     |  0.8950 |  0.2720 |
| R     |  0.9110 |  0.2520 |
| S     |  0.9080 |  0.2680 |
| T     |  0.7870 |  0.2640 |
| U     |  0.9090 |  0.2640 |
| V     |  0.9550 |  0.2640 |
| W     |  0.8950 |  0.2520 |
| X     |  0.8550 |  0.2810 |
| Y     |  0.8290 |  0.3140 |
| Z     |  0.9090 |  0.3280 |
| a     |  0.9520 |  0.2630 |
| b     |  0.9070 |  0.3160 |
| c     |  0.8280 |  0.2800 |
| d     |  0.9120 |  0.2950 |
| e     |  0.8900 |  0.2670 |
| f     |  0.6310 |  0.1620 |
| g     |  0.8720 |  0.2360 |
| h     |  0.8730 |  0.2330 |
| i     |  0.8180 |  0.2430 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| l     |  0.9310 |  0.2970 |
| y     |  0.9450 |  0.2150 |
| z     |  0.9160 |  0.1990 |