



## Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 02:04 PM UTC

PDB ID : 6XGF / pdb\_00006xgf  
EMDB ID : EMD-22181  
Title : Escherichia coli transcription-translation complex B (TTC-B) containing an  
30 nt long mRNA spacer, NusG, and fMet-tRNAs at E-site and P-site  
Authors : Molodtsov, V.; Wang, C.; Su, M.; Ebright, R.H.  
Deposited on : 2020-06-17  
Resolution : 5.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

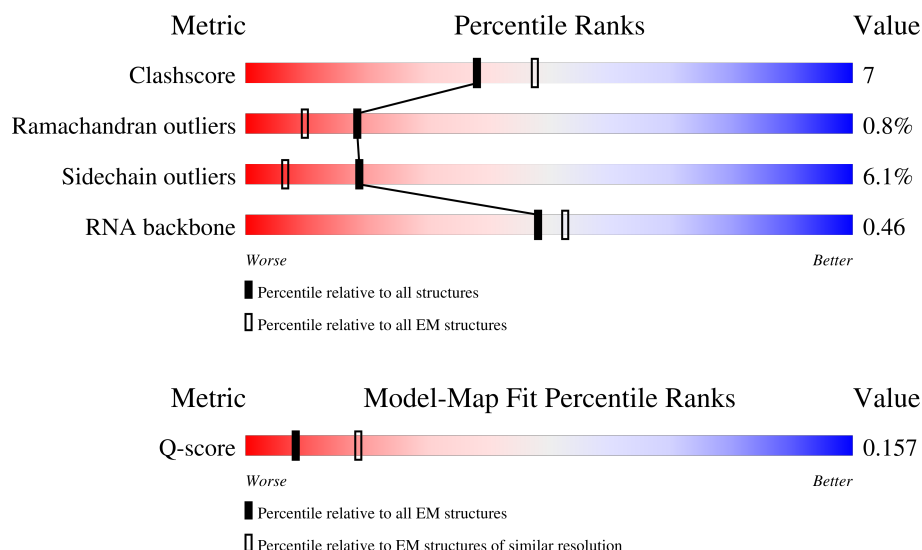
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 5.00 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                       | 1057 ( 4.50 - 5.50 )                                     |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 0     | 103    |                  |
| 2   | 1     | 110    |                  |
| 3   | 2     | 100    |                  |

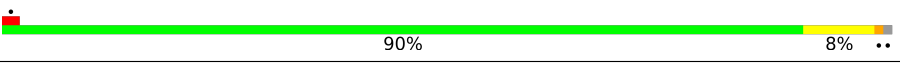
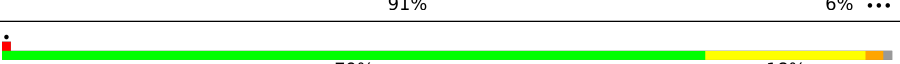
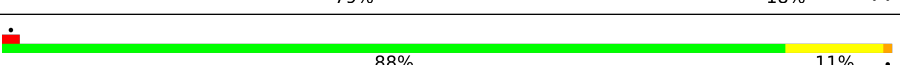
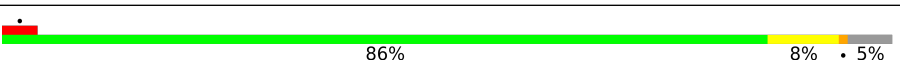
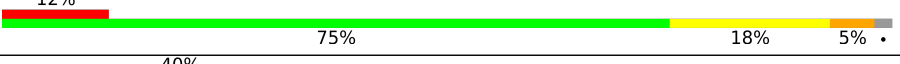
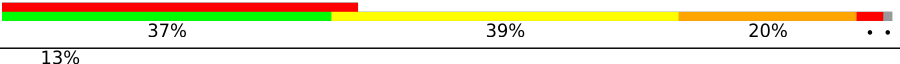
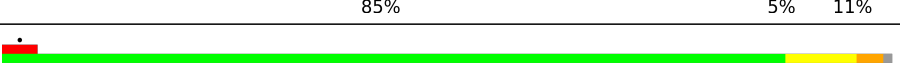
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | 3     | 104    |                  |
| 5   | 4     | 94     |                  |
| 6   | 5     | 36     |                  |
| 7   | 6     | 36     |                  |
| 8   | 7     | 45     |                  |
| 9   | 9     | 165    |                  |
| 10  | A     | 76     |                  |
| 10  | B     | 76     |                  |
| 11  | AA    | 1342   |                  |
| 12  | AB    | 181    |                  |
| 13  | AC    | 329    |                  |
| 13  | AD    | 329    |                  |
| 14  | AE    | 1407   |                  |
| 15  | AF    | 91     |                  |
| 16  | C     | 75     |                  |
| 17  | D     | 1542   |                  |
| 18  | E     | 87     |                  |
| 19  | F     | 71     |                  |
| 20  | G     | 241    |                  |
| 21  | H     | 557    |                  |
| 22  | I     | 233    |                  |
| 23  | J     | 206    |                  |
| 24  | K     | 167    |                  |
| 25  | L     | 135    |                  |
| 26  | M     | 179    |                  |

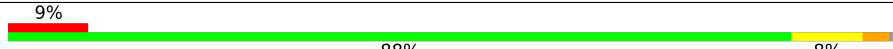
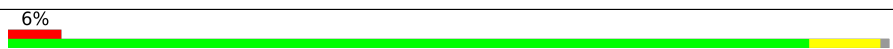
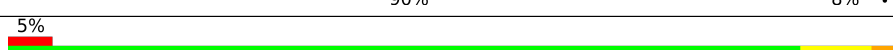
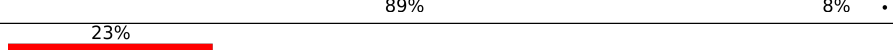
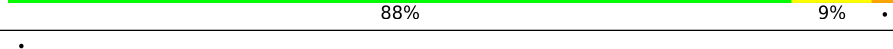
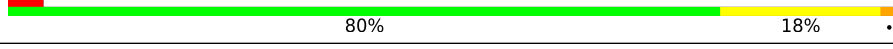
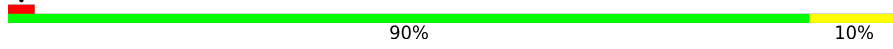
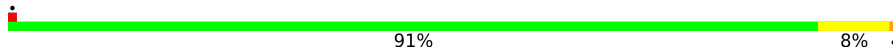
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 27  | N     | 130    |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

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 52  | m     | 46     |    |
| 53  | n     | 179    |    |
| 54  | o     | 65     |    |
| 55  | p     | 177    |    |
| 56  | q     | 38     |    |
| 57  | r     | 149    |    |
| 58  | s     | 142    |    |
| 59  | t     | 123    |    |
| 60  | u     | 144    |    |
| 61  | v     | 136    |    |
| 62  | w     | 127    |    |
| 63  | x     | 117    |    |
| 64  | y     | 115    |   |
| 65  | z     | 118    |  |

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

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

## 2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 276512 atoms, of which 99300 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L21.

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

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

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

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

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

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

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

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

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

- Molecule 6 is a DNA chain called NT DNA.

| Mol | Chain | Residues | Atoms |     |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|----|---------|-------|
| 6   | 5     | 23       | Total | C   | H   | N  | O   | P  | 0       | 0     |
|     |       |          | 732   | 225 | 260 | 87 | 137 | 23 |         |       |

- Molecule 7 is a DNA chain called T DNA.

| Mol | Chain | Residues | Atoms |     |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|----|---------|-------|
| 7   | 6     | 27       | Total | C   | H   | N  | O   | P  | 0       | 0     |
|     |       |          | 847   | 259 | 305 | 89 | 167 | 27 |         |       |

- Molecule 8 is a RNA chain called mRNA with 30 nt long spacer.

| Mol | Chain | Residues | Atoms |     |    |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|-----|----|---------|-------|
| 8   | 7     | 34       | Total | C   | H  | N  | O   | P  | 0       | 0     |
|     |       |          | 804   | 316 | 97 | 98 | 259 | 34 |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|---------|-------|
| 10  | A     | 76       | Total | C   | H   | N   | O   | P  | 0       | 0     |
|     |       |          | 2446  | 723 | 826 | 295 | 527 | 75 |         |       |
| 10  | B     | 76       | Total | C   | H   | N   | O   | P  | 0       | 0     |
|     |       |          | 2433  | 723 | 813 | 295 | 527 | 75 |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 11  | AA    | 1340     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10567 | 6631 | 1841 | 2052 | 43 |         |       |

- Molecule 12 is a protein called Transcription termination/antitermination protein NusG.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | AB    | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1392  | 881 | 249 | 255 | 7 |         |       |

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| AE    | 1384    | VAL      | MET    | conflict | UNP A0A4S1NBU2 |

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

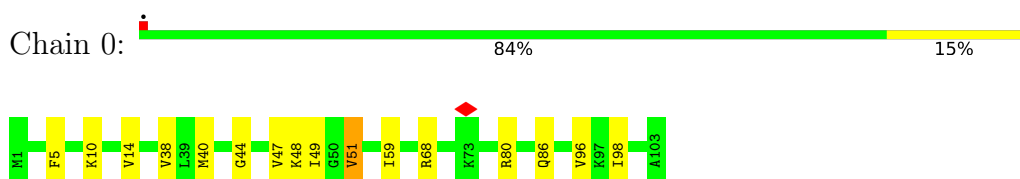
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 67  | AE    | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |



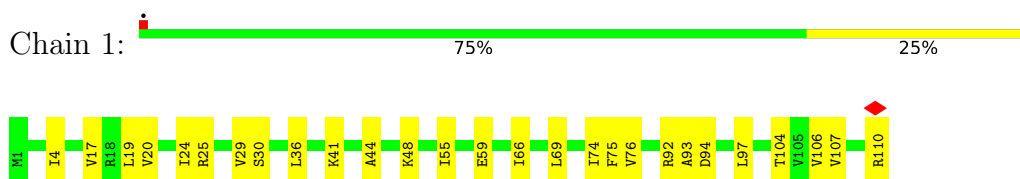
### 3 Residue-property plots [i](#)

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

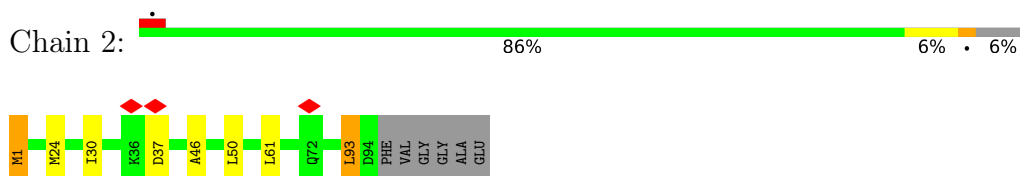
- Molecule 1: 50S ribosomal protein L21



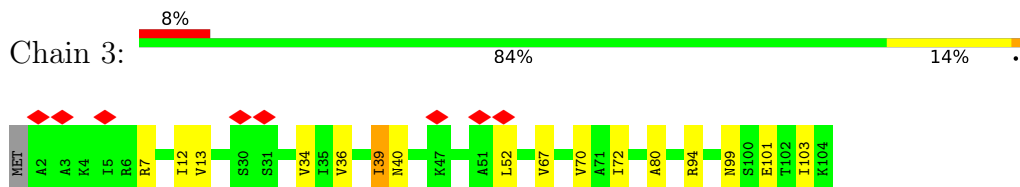
- Molecule 2: 50S ribosomal protein L22



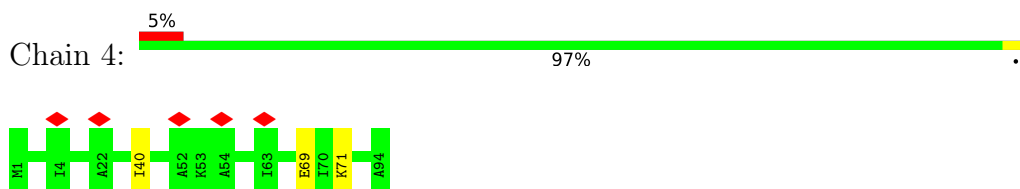
- Molecule 3: 50S ribosomal protein L23



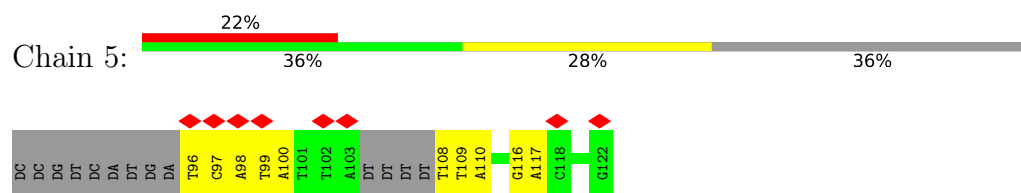
- Molecule 4: 50S ribosomal protein L24



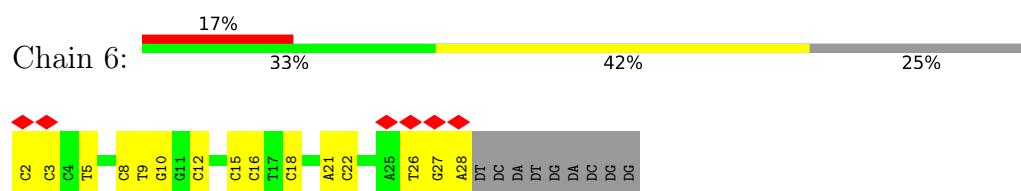
- Molecule 5: 50S ribosomal protein L25



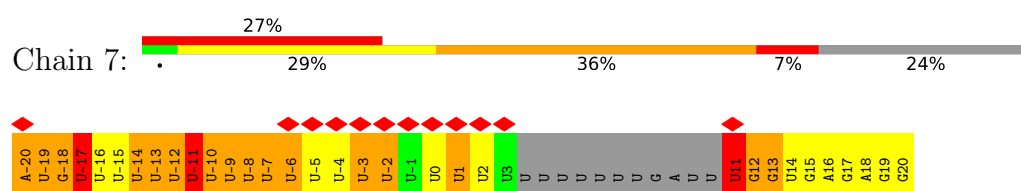
- Molecule 6: NT DNA



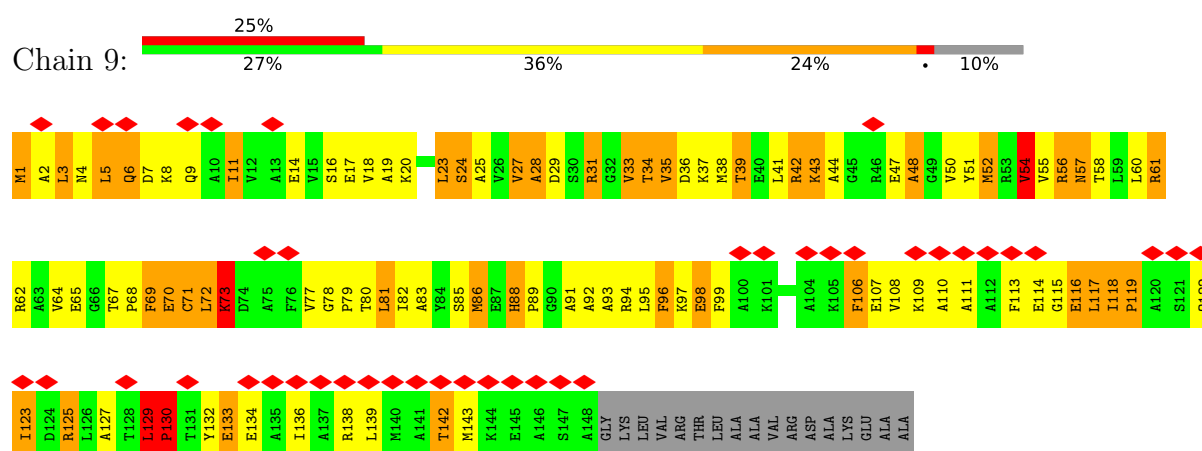
- Molecule 7: T DNA



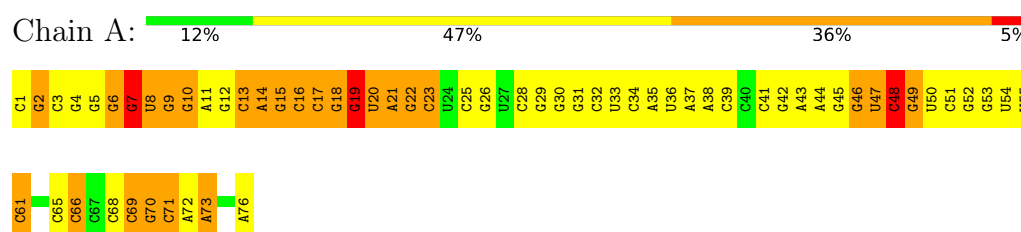
- Molecule 8: mRNA with 30 nt long spacer



- Molecule 9: 50S ribosomal protein L10

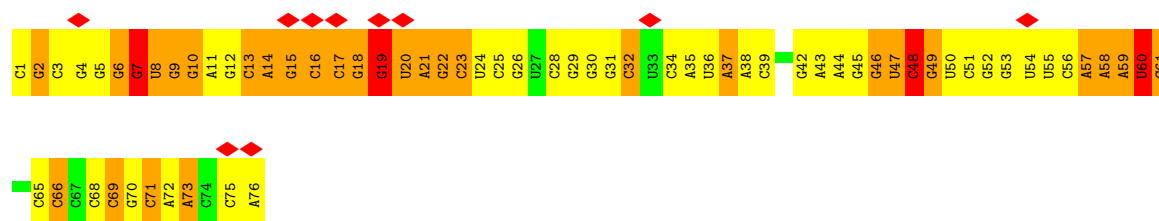


- Molecule 10: E-site and P-site tRNA (fMet)

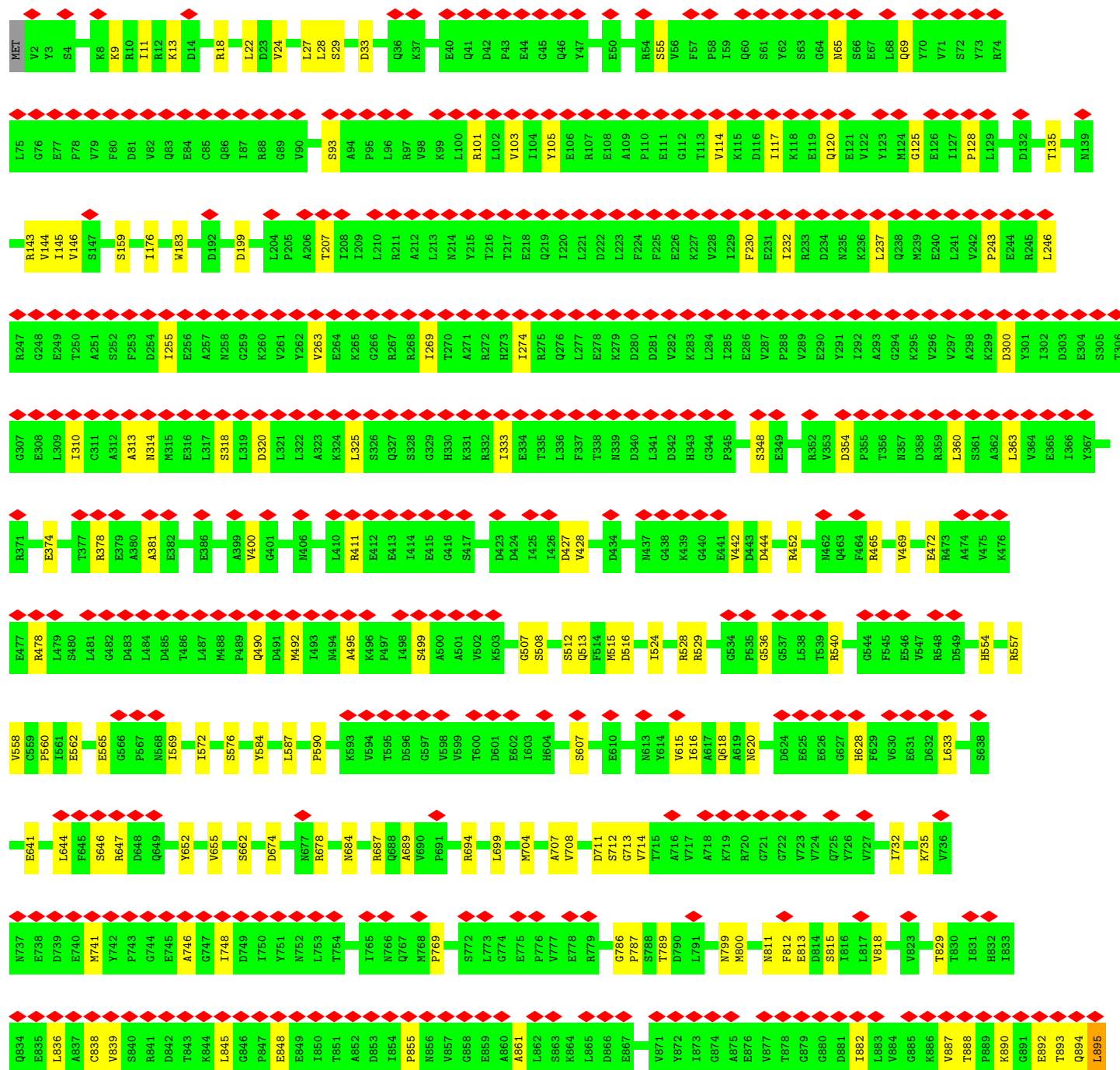
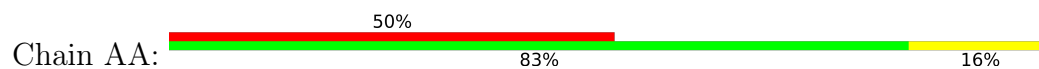


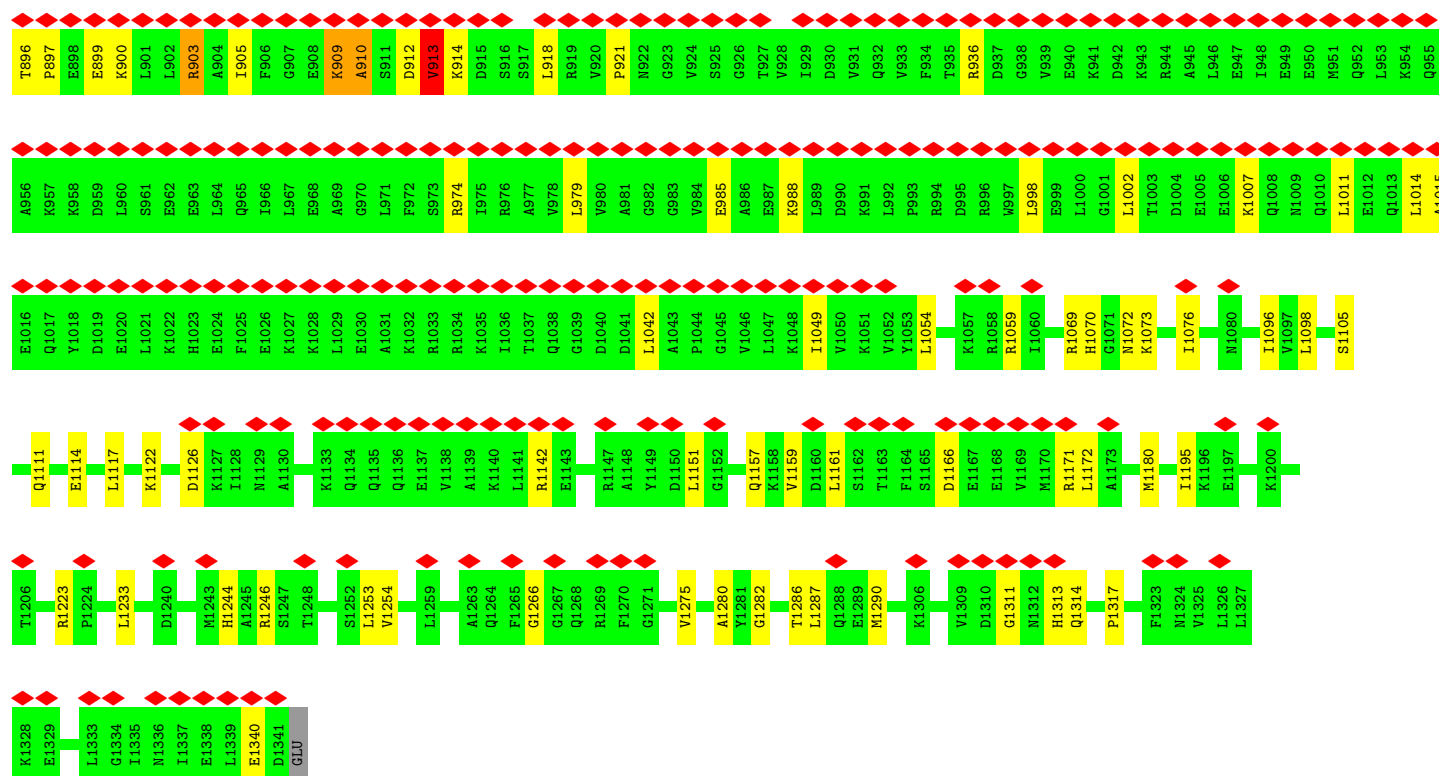
- Molecule 10: E-site and P-site tRNA (fMet)



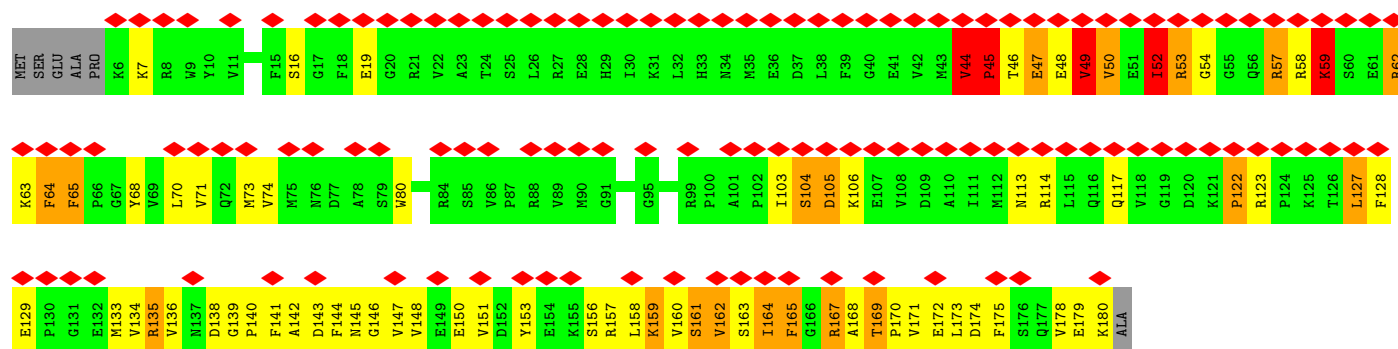
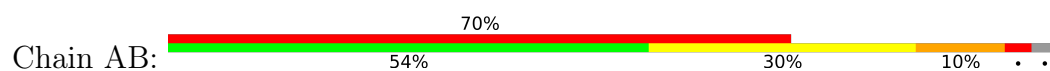


• Molecule 11: DNA-directed RNA polymerase subunit beta

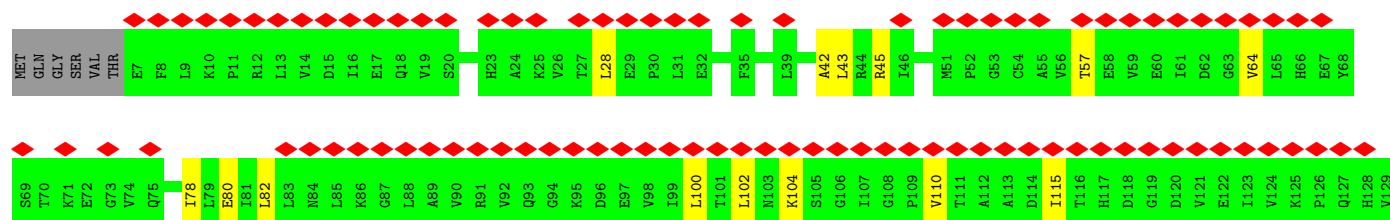


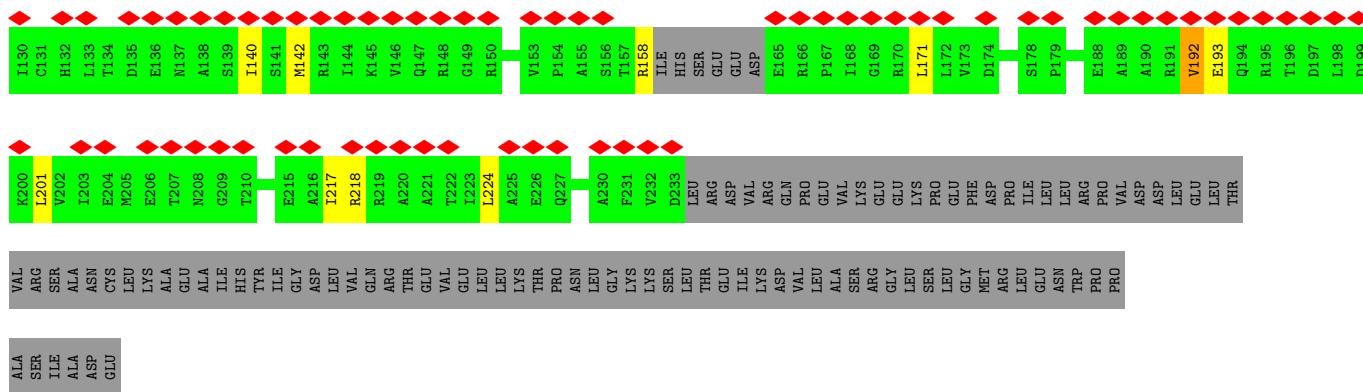


• Molecule 12: Transcription termination/antitermination protein NusG

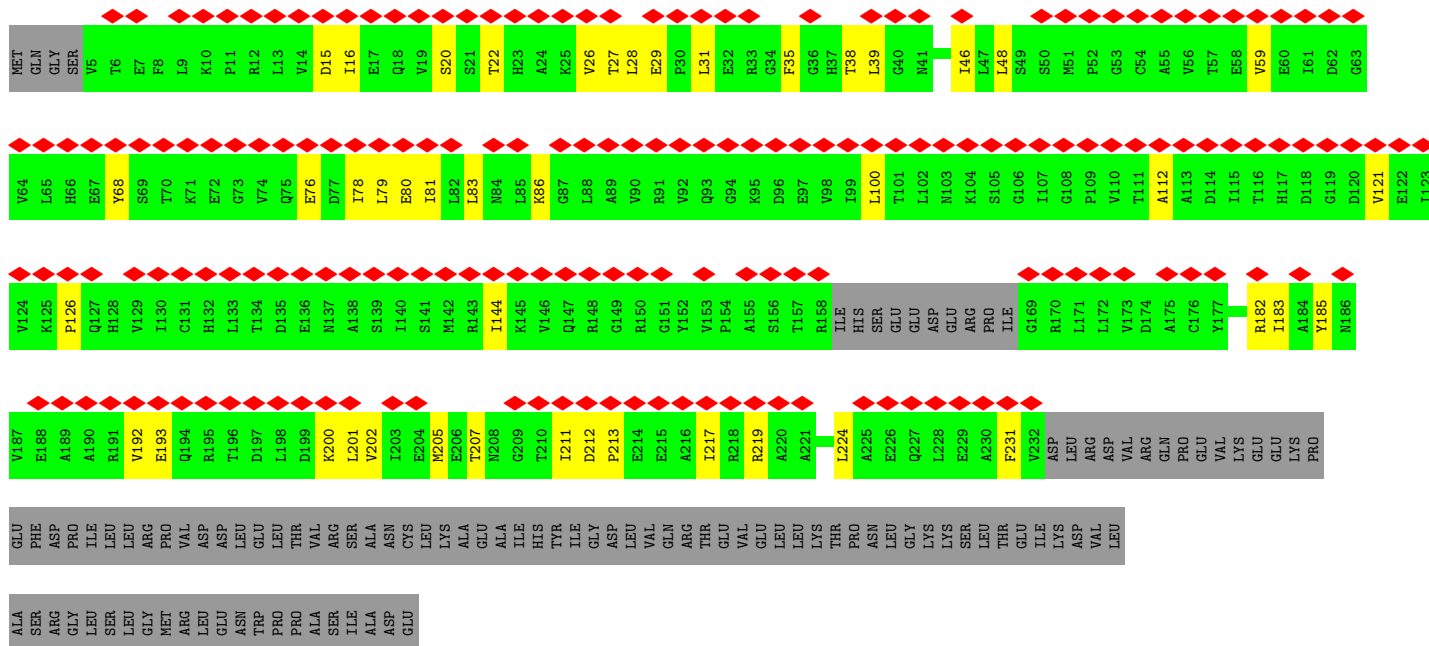


• Molecule 13: DNA-directed RNA polymerase subunit alpha

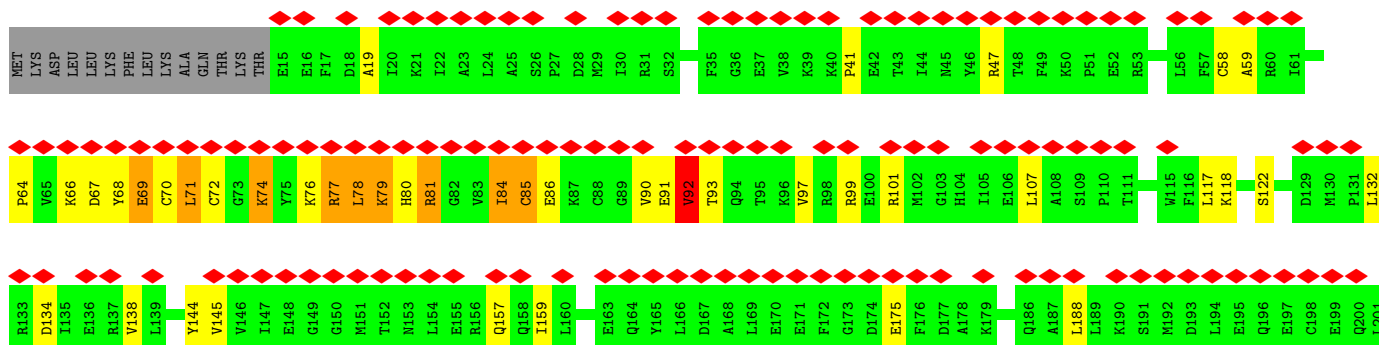
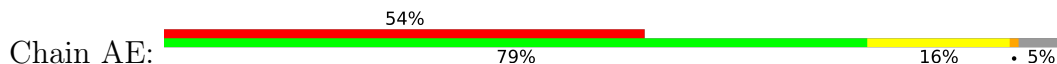


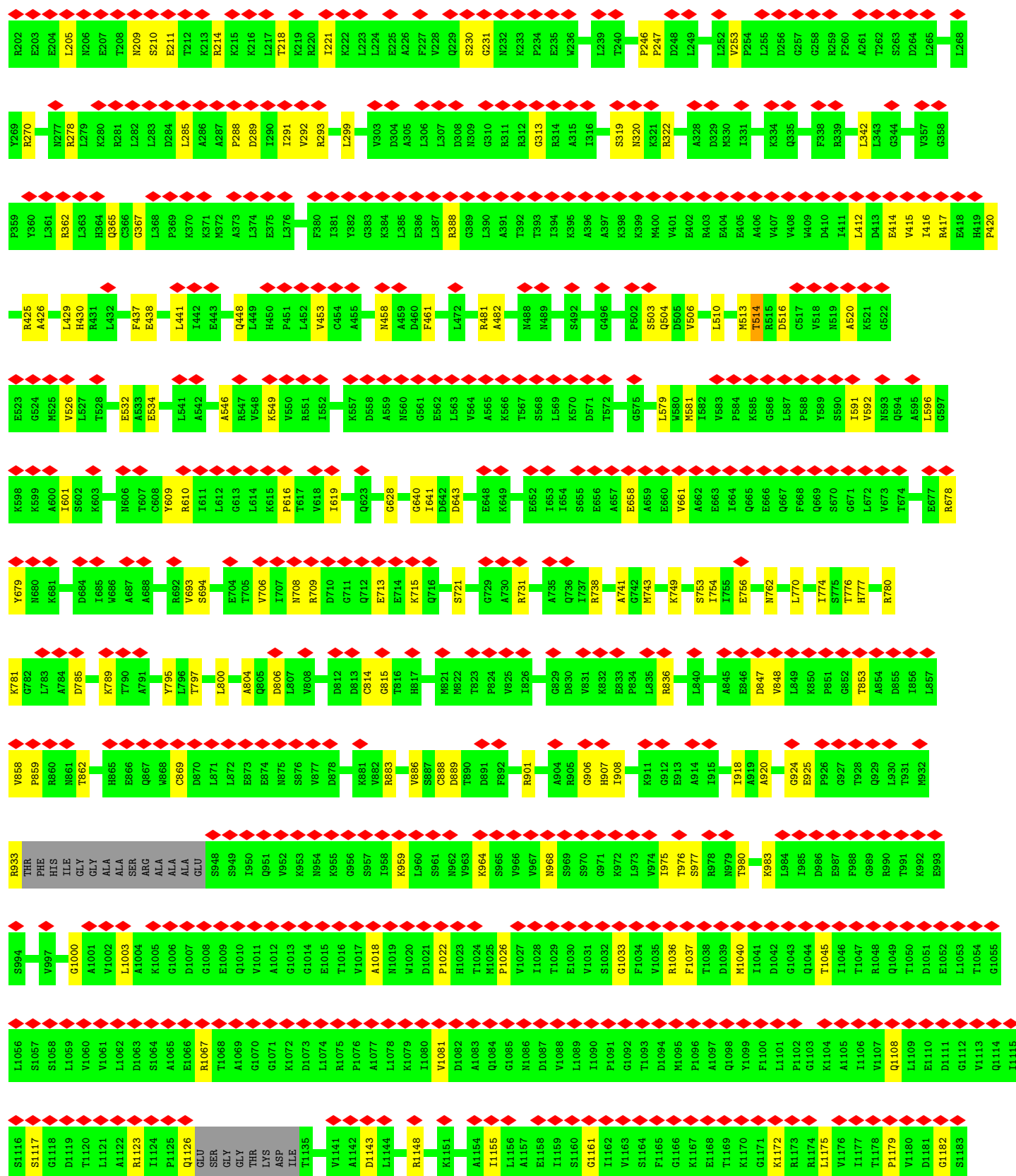


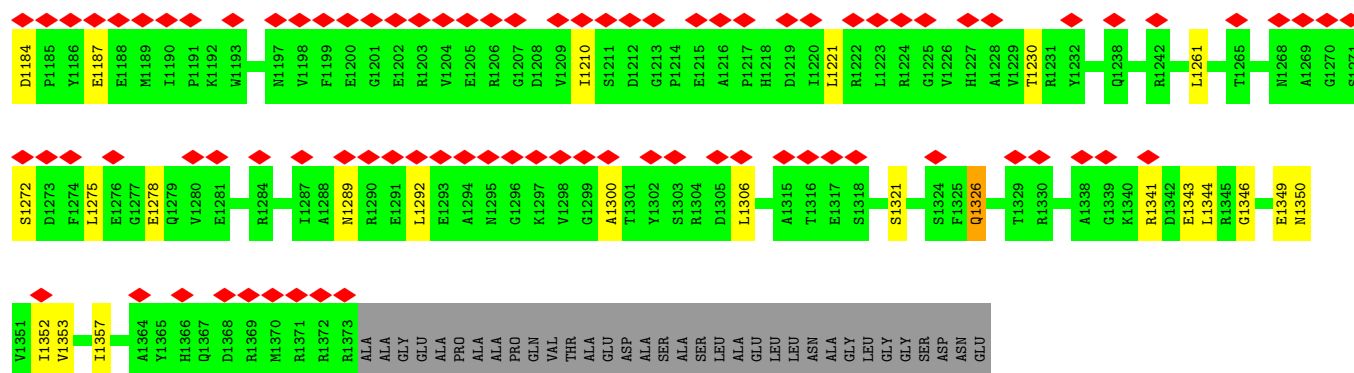
• Molecule 13: DNA-directed RNA polymerase subunit alpha



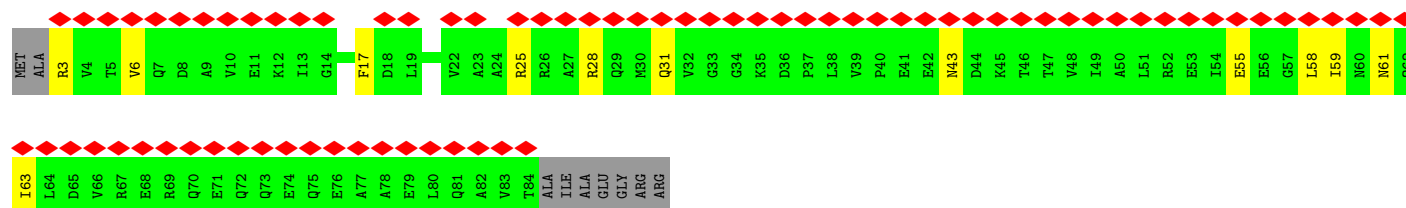
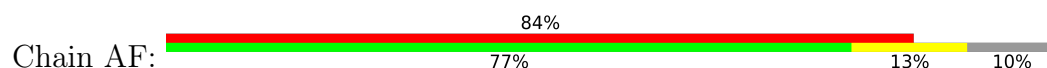
• Molecule 14: DNA-directed RNA polymerase subunit beta'



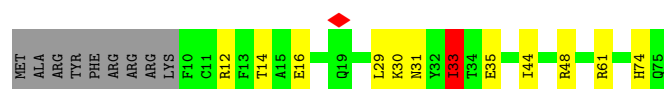




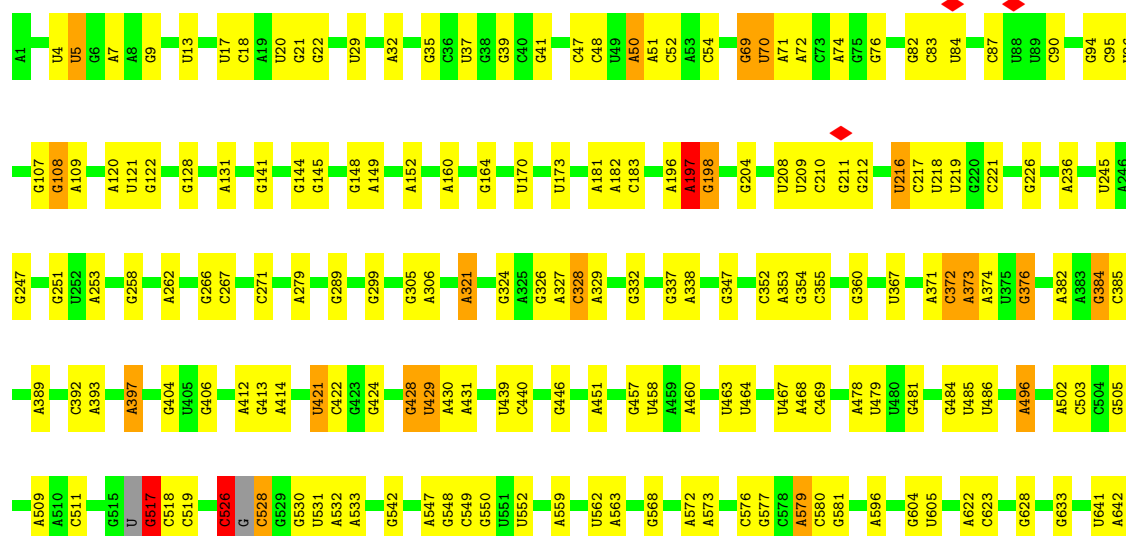
• Molecule 15: DNA-directed RNA polymerase subunit omega

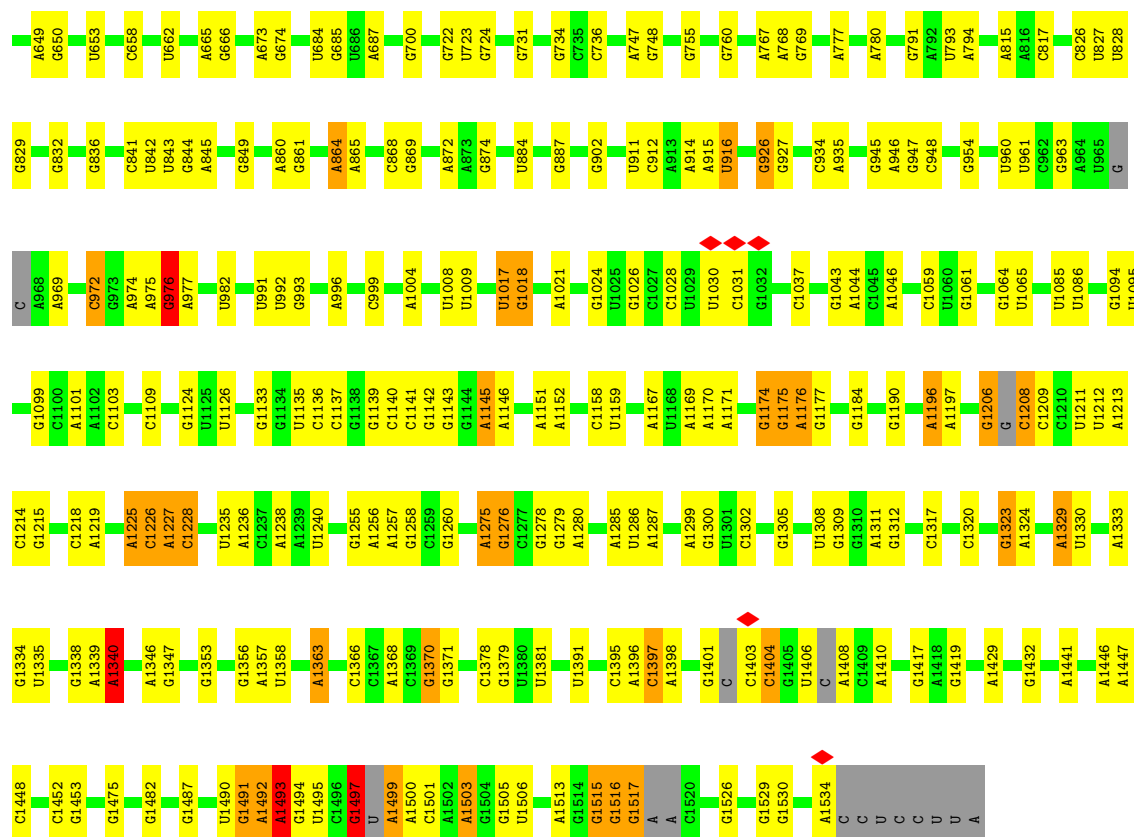


• Molecule 16: 30S ribosomal protein S18

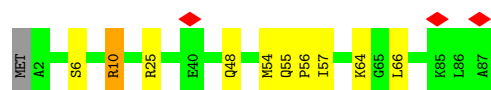
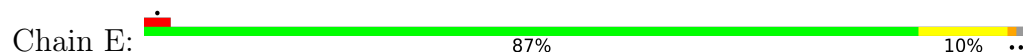


• Molecule 17: 16S rRNA

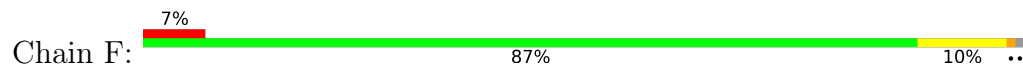




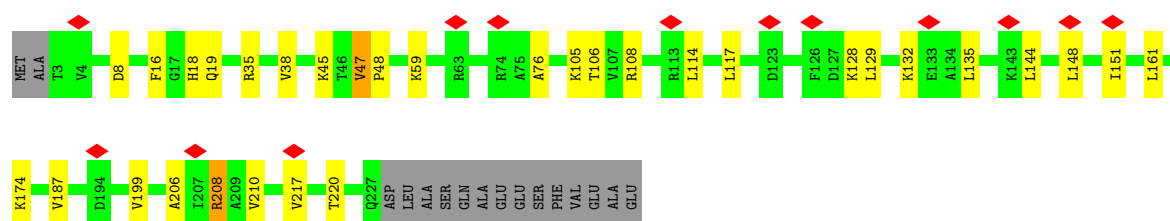
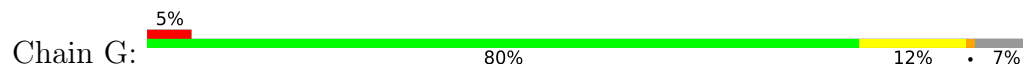
• Molecule 18: 30S ribosomal protein S20



• Molecule 19: 30S ribosomal protein S21

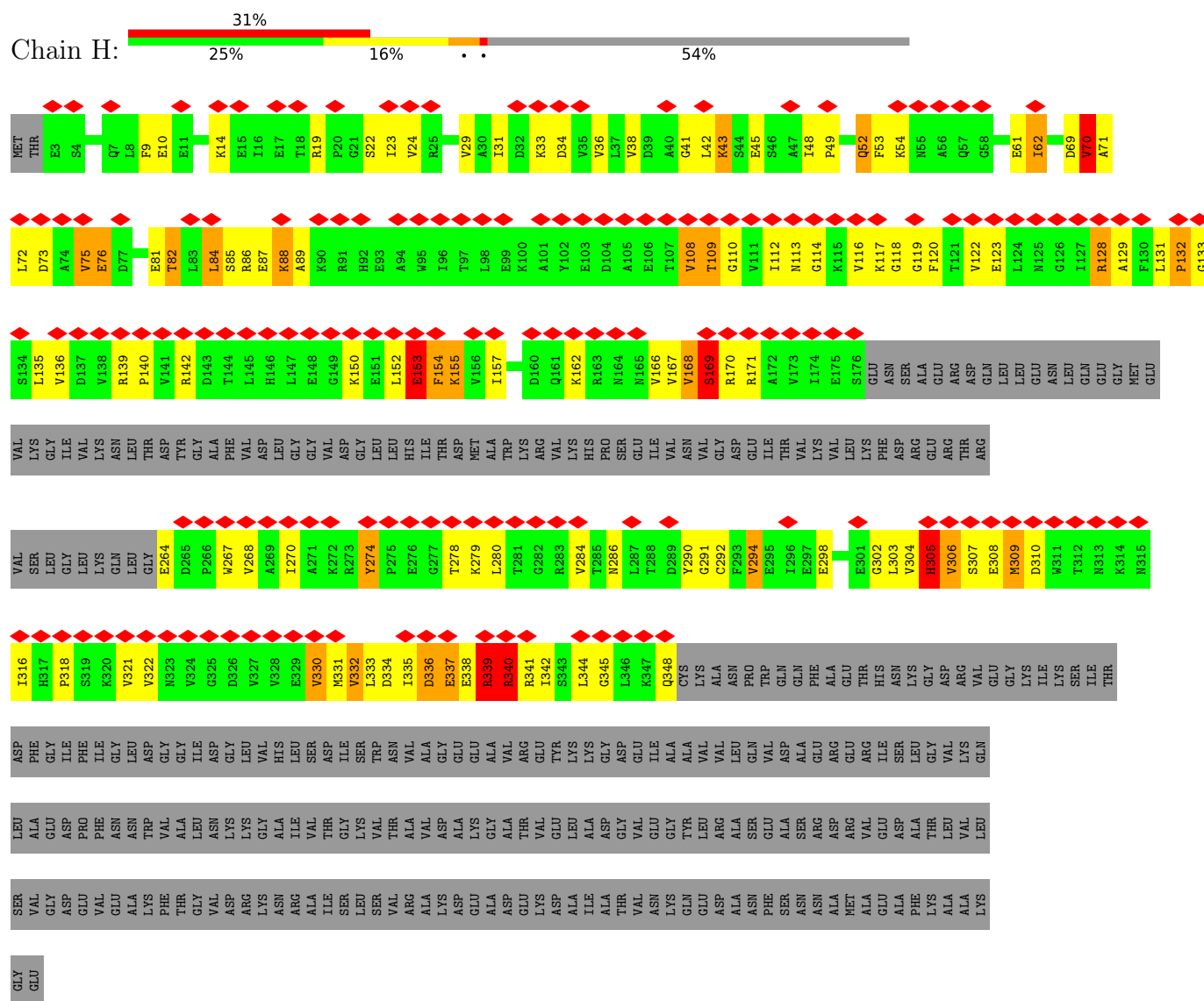


• Molecule 20: 30S ribosomal protein S2

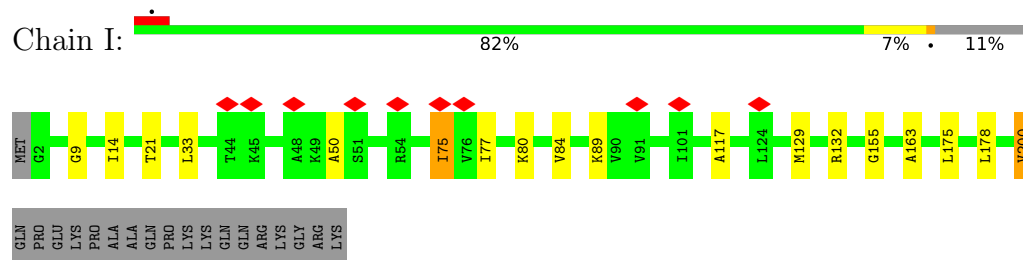




- Molecule 21: 30S ribosomal protein S1

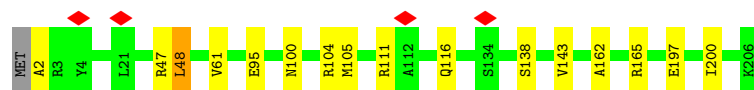


- Molecule 22: 30S ribosomal protein S3



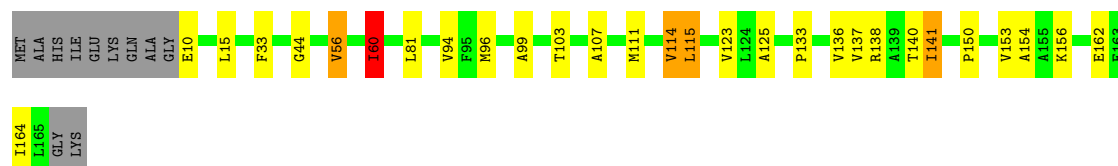
- Molecule 23: 30S ribosomal protein S4





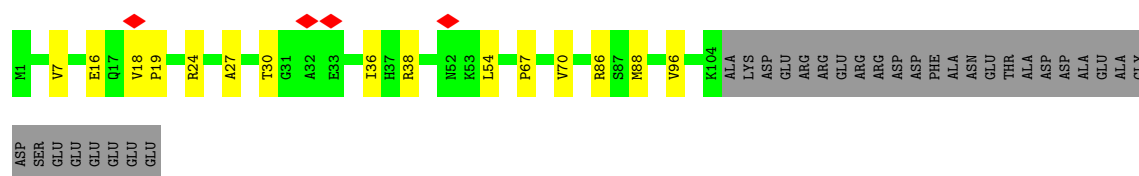
- Molecule 24: 30S ribosomal protein S5

Chain K: 76% 14% 7%



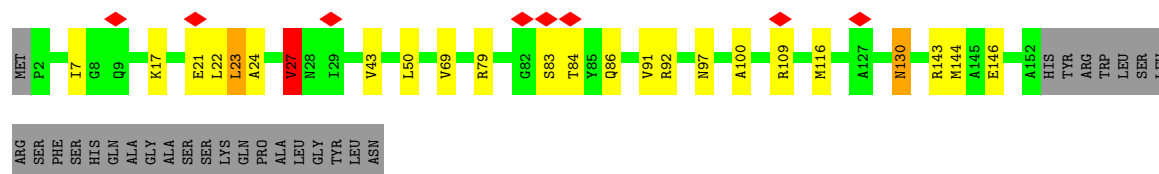
- Molecule 25: 30S ribosomal protein S6

Chain L: 66% 11% 23%



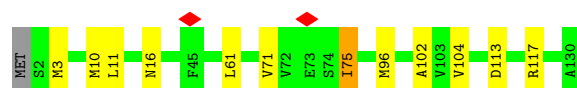
- Molecule 26: 30S ribosomal protein S7

Chain M: 71% 12% 16%



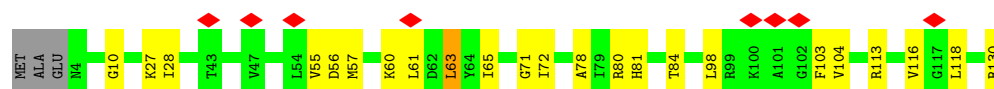
- Molecule 27: 30S ribosomal protein S8

Chain N: 90% 8% 2%

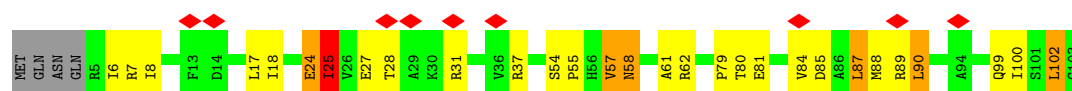


- Molecule 28: 30S ribosomal protein S9

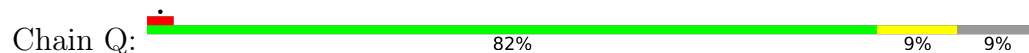
Chain O: 6% 80% 17%



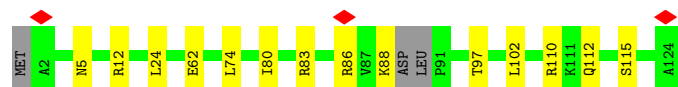
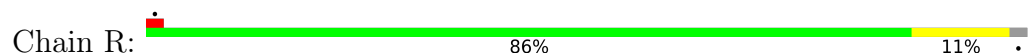
- Molecule 29: 30S ribosomal protein S10



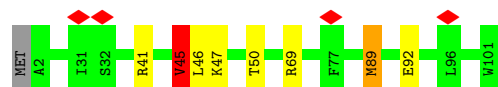
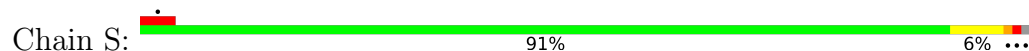
- Molecule 30: 30S ribosomal protein S11



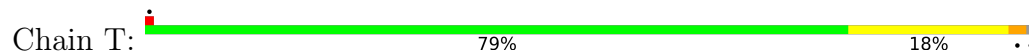
- Molecule 31: 30S ribosomal protein S12



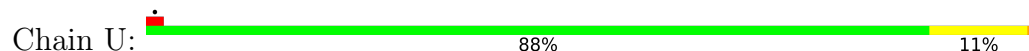
- Molecule 32: 30S ribosomal protein S14



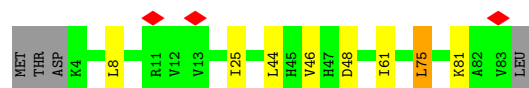
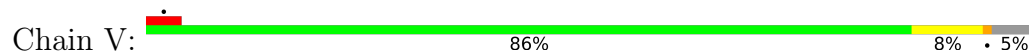
- Molecule 33: 30S ribosomal protein S15



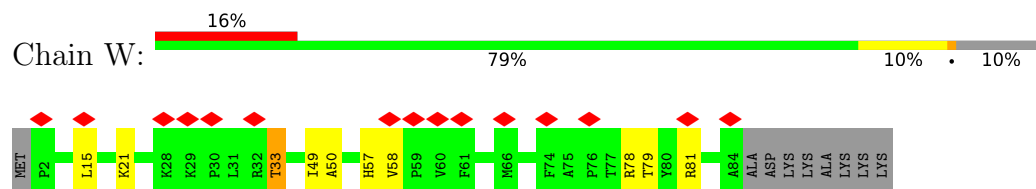
- Molecule 34: 30S ribosomal protein S16



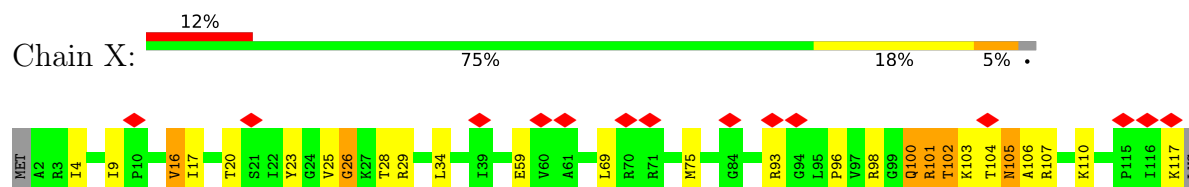
- Molecule 35: 30S ribosomal protein S17



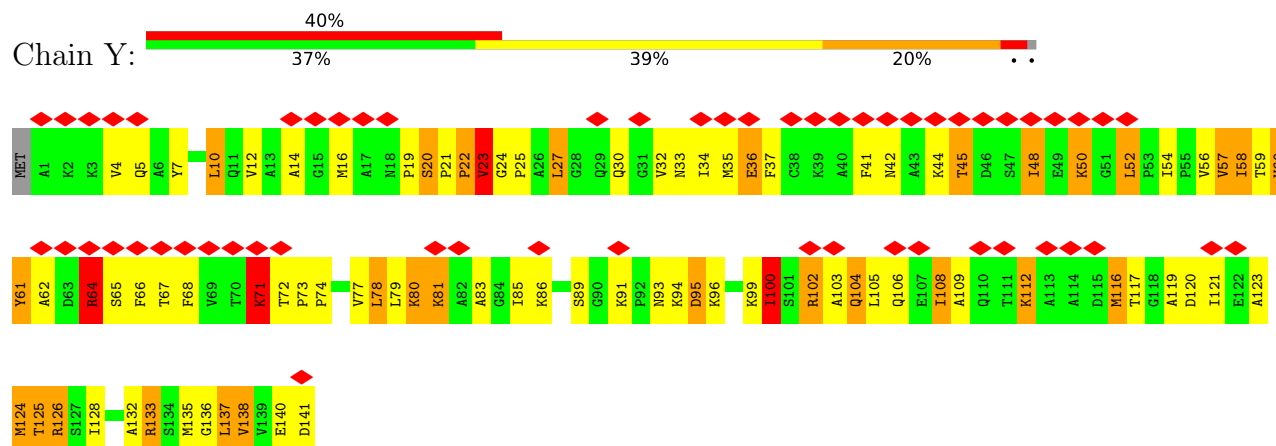
- Molecule 36: 30S ribosomal protein S19



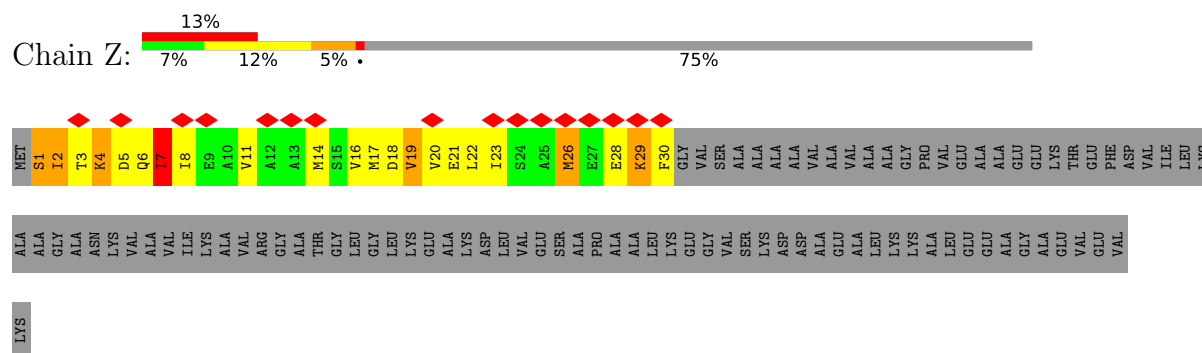
- Molecule 37: 30S ribosomal protein S13



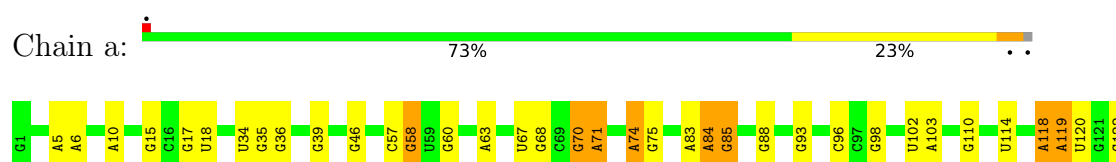
- Molecule 38: 50S ribosomal protein L11

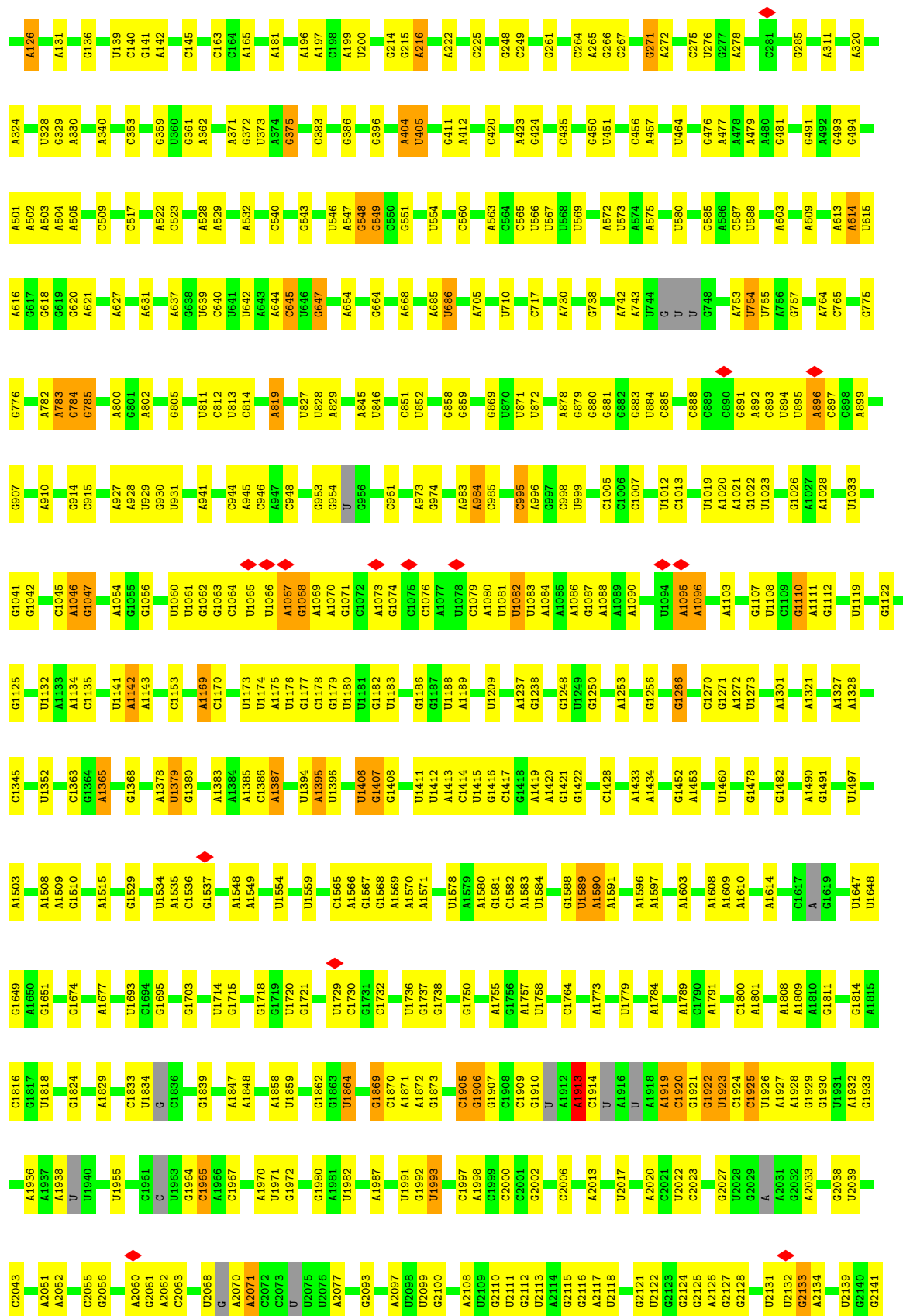


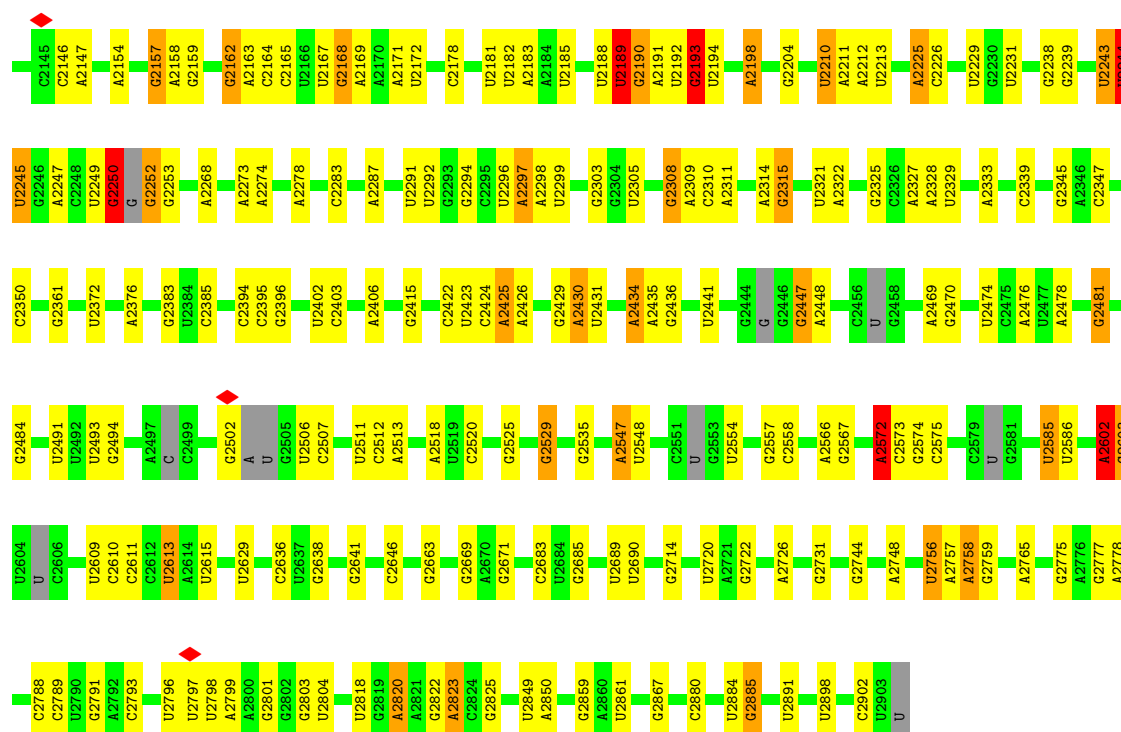
- Molecule 39: 50S ribosomal protein L7/L12



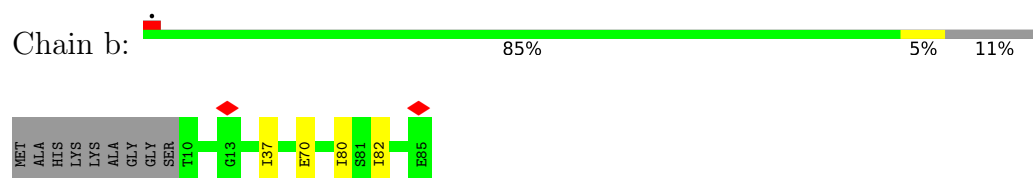
- Molecule 40: 23S rRNA



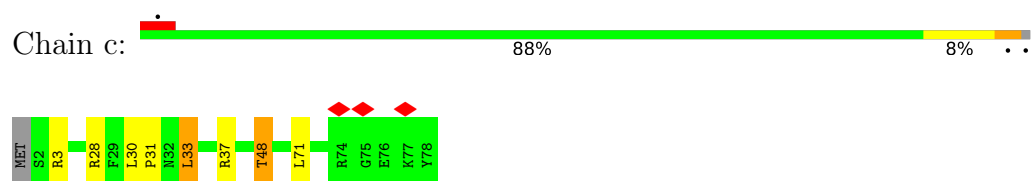




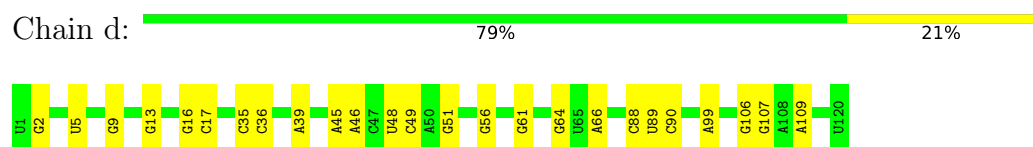
• Molecule 41: 50S ribosomal protein L27



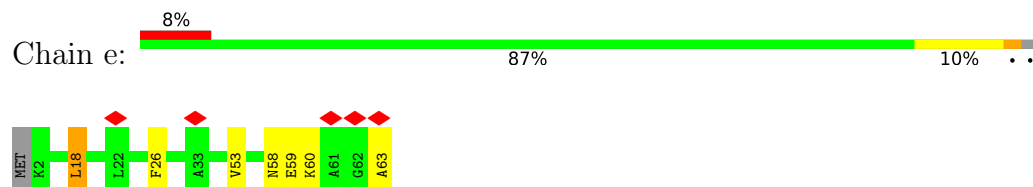
• Molecule 42: 50S ribosomal protein L28



• Molecule 43: 5S rRNA

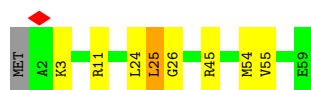


• Molecule 44: 50S ribosomal protein L29



- Molecule 45: 50S ribosomal protein L30

Chain f:  85% 12% ..



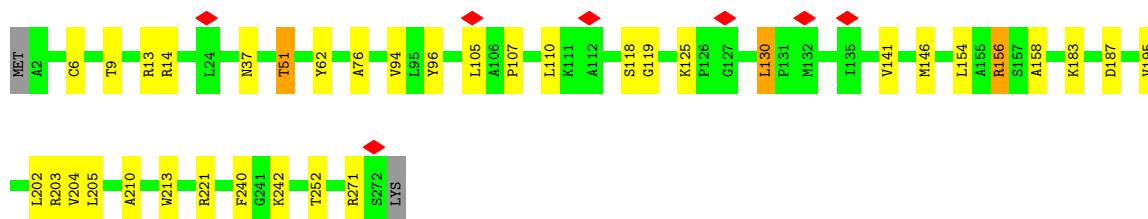
- Molecule 46: 50S ribosomal protein L31

Chain g:  19% 80% 13% 6%



- Molecule 47: 50S ribosomal protein L2

Chain h:  86% 12% ..



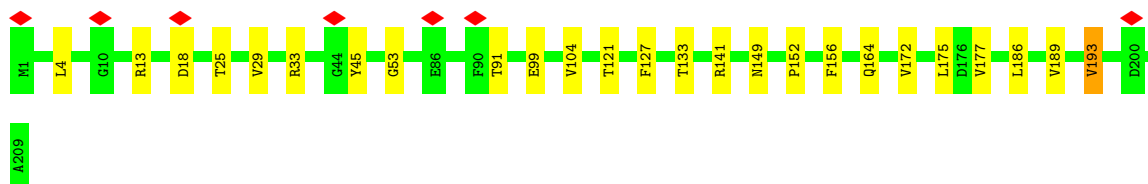
- Molecule 48: 50S ribosomal protein L32

Chain i:  79% 18% ..



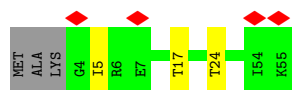
- Molecule 49: 50S ribosomal protein L3

Chain j:  88% 11%

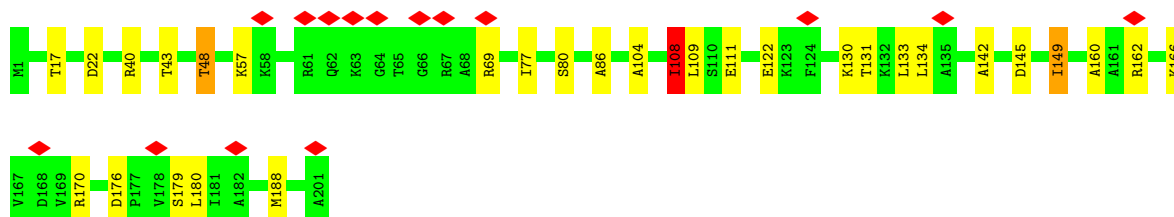
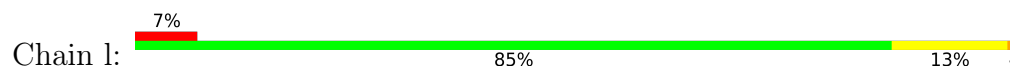


- Molecule 50: 50S ribosomal protein L33

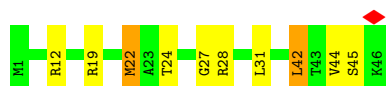
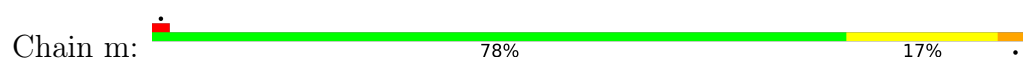
Chain k:  7% 89% 5% 5%



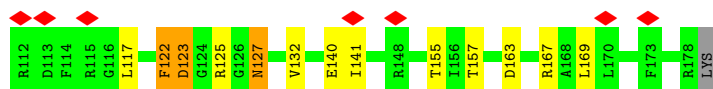
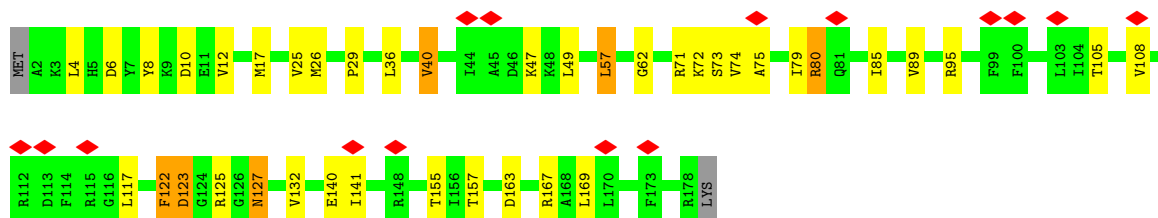
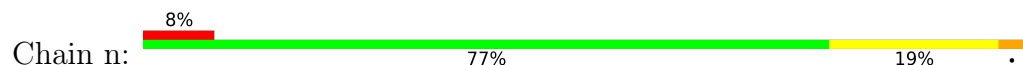
- Molecule 51: 50S ribosomal protein L4



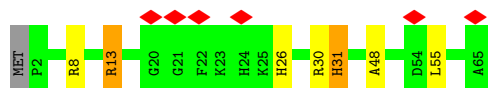
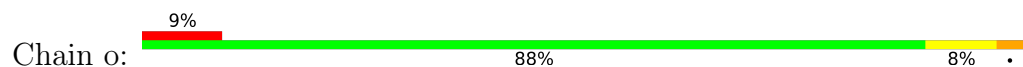
- Molecule 52: 50S ribosomal protein L34



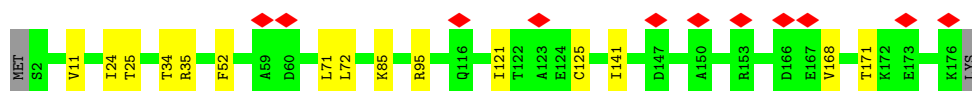
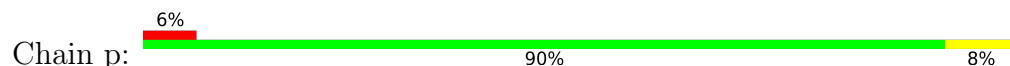
- Molecule 53: 50S ribosomal protein L5



- Molecule 54: 50S ribosomal protein L35

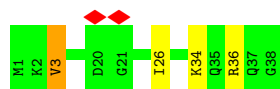
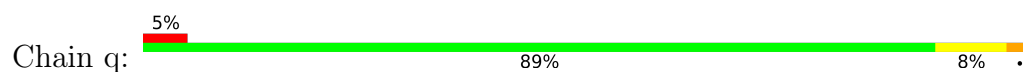


- Molecule 55: 50S ribosomal protein L6

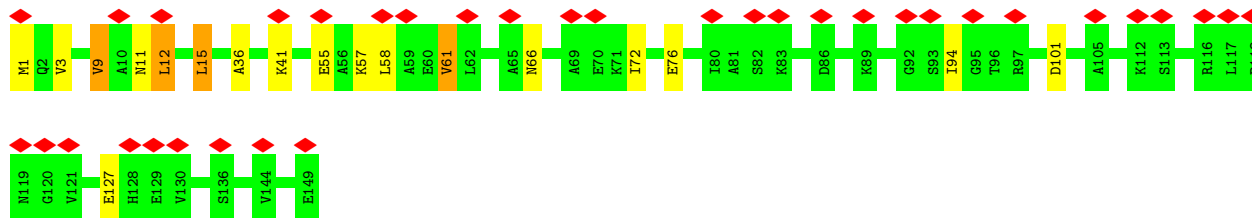
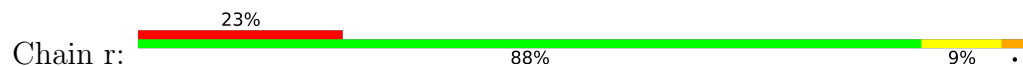


- Molecule 56: 50S ribosomal protein L36

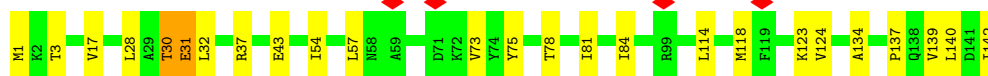
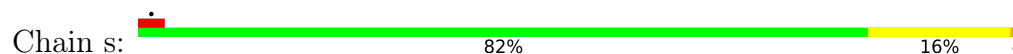




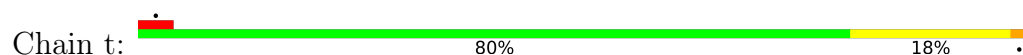
- Molecule 57: 50S ribosomal protein L9



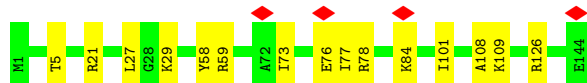
- Molecule 58: 50S ribosomal protein L13



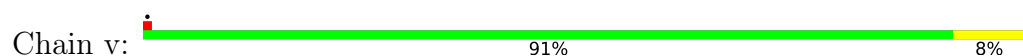
- Molecule 59: 50S ribosomal protein L14



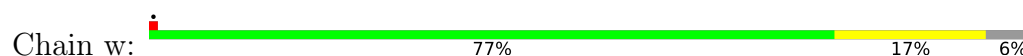
- Molecule 60: 50S ribosomal protein L15



- Molecule 61: 50S ribosomal protein L16



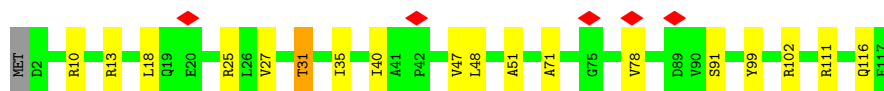
- Molecule 62: 50S ribosomal protein L17





- Molecule 63: 50S ribosomal protein L18

Chain x: 84% 15% ..



- Molecule 64: 50S ribosomal protein L19

Chain y: 5% 89% 10% .



- Molecule 65: 50S ribosomal protein L20

Chain z: 84% 14% ..



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 4617                                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TALOS ARCTICA                       | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 45                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.028                                   | Depositor |
| Minimum map value                    | -0.009                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.002                                   | Depositor |
| Recommended contour level            | 0.0062                                  | Depositor |
| Map size ( $\text{\AA}$ )            | 532.48, 532.48, 532.48                  | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.04, 1.04, 1.04                        | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | 0     | 0.49         | 0/829          | 0.74        | 0/1107          |
| 2   | 1     | 0.67         | 0/864          | 1.08        | 0/1156          |
| 3   | 2     | 0.54         | 0/752          | 0.89        | 0/1005          |
| 4   | 3     | 0.47         | 0/796          | 0.77        | 0/1062          |
| 5   | 4     | 0.52         | 0/766          | 0.88        | 0/1025          |
| 6   | 5     | 0.63         | 1/528 (0.2%)   | 0.55        | 0/810           |
| 7   | 6     | 0.55         | 1/603 (0.2%)   | 0.56        | 0/926           |
| 8   | 7     | 0.57         | 2/783 (0.3%)   | 0.89        | 4/1212 (0.3%)   |
| 9   | 9     | 1.15         | 3/1131 (0.3%)  | 1.30        | 4/1524 (0.3%)   |
| 10  | A     | 0.36         | 0/1810         | 0.72        | 2/2821 (0.1%)   |
| 10  | B     | 0.43         | 0/1810         | 0.87        | 9/2821 (0.3%)   |
| 11  | AA    | 0.39         | 0/10736        | 0.64        | 0/14487         |
| 12  | AB    | 1.00         | 2/1421 (0.1%)  | 1.10        | 4/1914 (0.2%)   |
| 13  | AC    | 0.37         | 0/1718         | 0.61        | 0/2328          |
| 13  | AD    | 0.32         | 0/1696         | 0.60        | 0/2298          |
| 14  | AE    | 0.38         | 0/10561        | 0.63        | 5/14258 (0.0%)  |
| 15  | AF    | 0.29         | 0/652          | 0.61        | 0/879           |
| 16  | C     | 0.66         | 0/553          | 1.14        | 2/743 (0.3%)    |
| 17  | D     | 0.39         | 9/36610 (0.0%) | 0.75        | 39/57091 (0.1%) |
| 18  | E     | 0.76         | 0/675          | 1.32        | 0/895           |
| 19  | F     | 0.71         | 0/597          | 1.20        | 0/792           |
| 20  | G     | 0.65         | 0/1791         | 1.08        | 1/2413 (0.0%)   |
| 21  | H     | 0.76         | 4/1746 (0.2%)  | 1.58        | 34/2382 (1.4%)  |
| 22  | I     | 0.58         | 0/1663         | 0.97        | 0/2241          |
| 23  | J     | 0.63         | 0/1665         | 1.08        | 0/2227          |
| 24  | K     | 0.63         | 1/1165 (0.1%)  | 1.06        | 2/1568 (0.1%)   |
| 25  | L     | 0.58         | 0/867          | 0.94        | 0/1171          |
| 26  | M     | 0.68         | 0/1195         | 1.19        | 3/1602 (0.2%)   |
| 27  | N     | 0.55         | 0/989          | 0.91        | 0/1326          |
| 28  | O     | 0.58         | 0/1034         | 1.02        | 1/1375 (0.1%)   |
| 29  | P     | 0.60         | 0/800          | 1.10        | 4/1082 (0.4%)   |
| 30  | Q     | 0.55         | 0/893          | 0.91        | 0/1205          |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 31  | R     | 0.49         | 0/952            | 0.81        | 0/1274            |
| 32  | S     | 0.64         | 0/817            | 1.11        | 1/1088 (0.1%)     |
| 33  | T     | 0.68         | 0/722            | 1.21        | 0/964             |
| 34  | U     | 0.58         | 0/659            | 0.99        | 0/884             |
| 35  | V     | 0.45         | 0/657            | 0.73        | 0/881             |
| 36  | W     | 0.50         | 0/680            | 0.83        | 0/915             |
| 37  | X     | 0.67         | 0/909            | 1.21        | 3/1215 (0.2%)     |
| 38  | Y     | 1.04         | 0/1046           | 1.09        | 1/1410 (0.1%)     |
| 39  | Z     | 1.02         | 0/227            | 1.12        | 0/304             |
| 40  | a     | 0.40         | 3/69247 (0.0%)   | 0.75        | 55/107985 (0.1%)  |
| 41  | b     | 0.51         | 0/589            | 0.76        | 0/779             |
| 42  | c     | 0.63         | 0/635            | 0.97        | 0/848             |
| 43  | d     | 0.37         | 0/2872           | 0.69        | 0/4478            |
| 44  | e     | 0.69         | 0/502            | 1.19        | 0/667             |
| 45  | f     | 0.62         | 0/452            | 1.02        | 0/605             |
| 46  | g     | 0.55         | 0/531            | 0.99        | 1/709 (0.1%)      |
| 47  | h     | 0.54         | 0/2121           | 0.85        | 0/2852            |
| 48  | i     | 0.52         | 0/450            | 0.94        | 0/599             |
| 49  | j     | 0.59         | 0/1586           | 0.87        | 0/2134            |
| 50  | k     | 0.46         | 0/433            | 0.80        | 0/576             |
| 51  | l     | 0.61         | 0/1571           | 1.03        | 1/2113 (0.0%)     |
| 52  | m     | 0.68         | 0/380            | 1.22        | 0/498             |
| 53  | n     | 0.62         | 0/1434           | 1.18        | 10/1926 (0.5%)    |
| 54  | o     | 0.63         | 0/513            | 1.10        | 1/676 (0.1%)      |
| 55  | p     | 0.58         | 0/1333           | 0.89        | 0/1805            |
| 56  | q     | 0.50         | 0/303            | 0.88        | 0/397             |
| 57  | r     | 0.63         | 0/1122           | 0.97        | 1/1515 (0.1%)     |
| 58  | s     | 0.68         | 0/1152           | 1.02        | 2/1551 (0.1%)     |
| 59  | t     | 0.57         | 0/955            | 0.88        | 0/1279            |
| 60  | u     | 0.55         | 0/1062           | 0.96        | 1/1413 (0.1%)     |
| 61  | v     | 0.59         | 0/1093           | 0.97        | 0/1460            |
| 62  | w     | 0.67         | 0/964            | 1.13        | 0/1289            |
| 63  | x     | 0.61         | 0/902            | 1.09        | 0/1209            |
| 64  | y     | 0.52         | 0/929            | 0.79        | 0/1242            |
| 65  | z     | 0.80         | 0/960            | 1.25        | 0/1278            |
| All | All   | 0.48         | 26/190459 (0.0%) | 0.82        | 191/280564 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 10  | A     | 0                   | 2                   |
| 10  | B     | 0                   | 2                   |
| 11  | AA    | 0                   | 1                   |
| 12  | AB    | 0                   | 1                   |
| 13  | AC    | 0                   | 1                   |
| 13  | AD    | 0                   | 1                   |
| 14  | AE    | 0                   | 4                   |
| 21  | H     | 0                   | 3                   |
| 37  | X     | 0                   | 1                   |
| All | All   | 0                   | 16                  |

All (26) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 9   | 9     | 130  | PRO  | N-CA   | 18.21  | 1.70        | 1.47     |
| 12  | AB    | 45   | PRO  | N-CA   | 18.17  | 1.70        | 1.47     |
| 21  | H     | 169  | SER  | N-CA   | 11.79  | 1.61        | 1.46     |
| 17  | D     | 1516 | G    | O3'-P  | -10.72 | 1.45        | 1.61     |
| 17  | D     | 1339 | A    | O3'-P  | 8.45   | 1.73        | 1.61     |
| 8   | 7     | 19   | G    | C1'-N9 | -7.50  | 1.36        | 1.48     |
| 6   | 5     | 109  | DT   | O3'-P  | 7.06   | 1.71        | 1.61     |
| 8   | 7     | -19  | U    | C1'-N1 | 7.04   | 1.59        | 1.48     |
| 21  | H     | 88   | LYS  | N-CA   | 7.04   | 1.55        | 1.46     |
| 17  | D     | 145  | G    | O3'-P  | 6.75   | 1.71        | 1.61     |
| 17  | D     | 196  | A    | O3'-P  | 6.63   | 1.71        | 1.61     |
| 21  | H     | 168  | VAL  | C-N    | 6.47   | 1.42        | 1.33     |
| 17  | D     | 1275 | A    | O3'-P  | 6.22   | 1.70        | 1.61     |
| 40  | a     | 2434 | A    | O3'-P  | 6.04   | 1.70        | 1.61     |
| 17  | D     | 1515 | G    | O3'-P  | -5.82  | 1.52        | 1.61     |
| 21  | H     | 88   | LYS  | CA-C   | 5.78   | 1.60        | 1.52     |
| 17  | D     | 1395 | C    | O3'-P  | 5.76   | 1.69        | 1.61     |
| 17  | D     | 1490 | U    | O3'-P  | 5.45   | 1.69        | 1.61     |
| 7   | 6     | 10   | DG   | C1'-N9 | -5.37  | 1.35        | 1.46     |
| 17  | D     | 1492 | A    | O3'-P  | 5.29   | 1.69        | 1.61     |
| 40  | a     | 1905 | C    | O3'-P  | 5.28   | 1.69        | 1.61     |
| 40  | a     | 2167 | U    | O3'-P  | 5.20   | 1.69        | 1.61     |
| 12  | AB    | 44   | VAL  | C-N    | 5.13   | 1.45        | 1.33     |
| 9   | 9     | 129  | LEU  | C-N    | 5.12   | 1.45        | 1.33     |
| 9   | 9     | 116  | GLU  | N-CA   | 5.08   | 1.49        | 1.46     |
| 24  | K     | 56   | VAL  | CA-CB  | 5.05   | 1.57        | 1.54     |

All (191) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 17  | D     | 1516 | G    | O3'-P-O5'   | 17.46  | 130.20      | 104.00   |
| 21  | H     | 88   | LYS  | CA-C-N      | 16.92  | 143.55      | 120.38   |
| 21  | H     | 88   | LYS  | C-N-CA      | 16.92  | 143.55      | 120.38   |
| 10  | B     | 29   | G    | C3'-C2'-O2' | 15.99  | 134.68      | 110.70   |
| 12  | AB    | 44   | VAL  | CA-C-N      | 15.89  | 139.70      | 119.84   |
| 12  | AB    | 44   | VAL  | C-N-CA      | 15.89  | 139.70      | 119.84   |
| 9   | 9     | 129  | LEU  | CA-C-N      | 15.84  | 139.64      | 119.84   |
| 9   | 9     | 129  | LEU  | C-N-CA      | 15.84  | 139.64      | 119.84   |
| 17  | D     | 1516 | G    | P-O3'-C3'   | -15.53 | 96.90       | 120.20   |
| 21  | H     | 332  | VAL  | N-CA-C      | 13.64  | 124.54      | 110.62   |
| 21  | H     | 169  | SER  | N-CA-C      | 12.74  | 137.94      | 110.80   |
| 21  | H     | 330  | VAL  | N-CA-C      | 12.17  | 126.91      | 109.51   |
| 21  | H     | 305  | HIS  | N-CA-C      | 11.95  | 131.09      | 111.37   |
| 40  | a     | 2244 | U    | C1'-C2'-O2' | -9.79  | 93.72       | 108.40   |
| 53  | n     | 73   | SER  | N-CA-CB     | -9.57  | 94.58       | 110.47   |
| 17  | D     | 1206 | G    | C4'-C3'-O3' | 9.55   | 127.33      | 113.00   |
| 29  | P     | 54   | SER  | CA-C-N      | 9.35   | 129.04      | 118.85   |
| 29  | P     | 54   | SER  | C-N-CA      | 9.35   | 129.04      | 118.85   |
| 40  | a     | 2250 | G    | C4'-C3'-O3' | -9.23  | 95.55       | 109.40   |
| 17  | D     | 1401 | G    | C4'-C3'-O3' | 8.85   | 126.28      | 113.00   |
| 17  | D     | 428  | G    | C4'-C3'-O3' | 8.71   | 122.47      | 109.40   |
| 12  | AB    | 45   | PRO  | CA-N-CD     | -8.68  | 99.84       | 112.00   |
| 8   | 7     | -20  | A    | O3'-P-O5'   | -8.62  | 91.08       | 104.00   |
| 9   | 9     | 130  | PRO  | CA-N-CD     | -8.61  | 99.95       | 112.00   |
| 21  | H     | 339  | ARG  | CA-C-N      | 8.55   | 137.88      | 121.54   |
| 21  | H     | 339  | ARG  | C-N-CA      | 8.55   | 137.88      | 121.54   |
| 32  | S     | 45   | VAL  | N-CA-CB     | 8.46   | 120.45      | 110.55   |
| 17  | D     | 1515 | G    | O3'-P-O5'   | -8.46  | 91.31       | 104.00   |
| 40  | a     | 2296 | U    | C4'-C3'-O3' | 8.40   | 122.01      | 109.40   |
| 40  | a     | 404  | A    | C2'-C3'-O3' | 8.35   | 122.02      | 109.50   |
| 29  | P     | 57   | VAL  | N-CA-C      | 8.29   | 120.04      | 107.77   |
| 8   | 7     | -17  | U    | C2'-C3'-O3' | 8.26   | 121.89      | 109.50   |
| 17  | D     | 197  | A    | C2'-C3'-O3' | 8.20   | 121.79      | 109.50   |
| 40  | a     | 2252 | G    | N9-C1'-C2'  | -8.15  | 99.77       | 112.00   |
| 17  | D     | 1401 | G    | N9-C1'-C2'  | -7.92  | 100.12      | 112.00   |
| 40  | a     | 2425 | A    | C2'-C3'-O3' | 7.83   | 121.25      | 109.50   |
| 21  | H     | 155  | LYS  | CA-C-N      | -7.77  | 110.94      | 121.66   |
| 21  | H     | 155  | LYS  | C-N-CA      | -7.77  | 110.94      | 121.66   |
| 40  | a     | 2071 | A    | C4'-C3'-O3' | -7.73  | 101.41      | 113.00   |
| 21  | H     | 168  | VAL  | CA-C-N      | 7.66   | 136.17      | 121.54   |
| 21  | H     | 168  | VAL  | C-N-CA      | 7.66   | 136.17      | 121.54   |
| 53  | n     | 75   | ALA  | CA-C-N      | 7.62   | 129.67      | 120.14   |
| 53  | n     | 75   | ALA  | C-N-CA      | 7.62   | 129.67      | 120.14   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | D     | 1493 | A    | C2'-C3'-O3' | 7.62  | 125.13      | 113.70   |
| 21  | H     | 84   | LEU  | N-CA-C      | 7.62  | 120.99      | 110.24   |
| 21  | H     | 52   | GLN  | N-CA-C      | -7.61 | 104.14      | 113.50   |
| 17  | D     | 1499 | A    | N9-C1'-C2'  | -7.58 | 100.62      | 112.00   |
| 37  | X     | 102  | THR  | CB-CA-C     | 7.57  | 123.40      | 110.84   |
| 17  | D     | 1339 | A    | P-O3'-C3'   | 7.56  | 131.54      | 120.20   |
| 24  | K     | 60   | ILE  | N-CA-CB     | 7.53  | 119.36      | 110.55   |
| 17  | D     | 528  | C    | N1-C1'-C2'  | -7.51 | 100.74      | 112.00   |
| 21  | H     | 336  | ASP  | CB-CA-C     | -7.45 | 98.64       | 110.79   |
| 53  | n     | 73   | SER  | CB-CA-C     | 7.42  | 122.88      | 110.79   |
| 24  | K     | 56   | VAL  | O-C-N       | 7.39  | 125.15      | 120.42   |
| 10  | B     | 28   | C    | P-O3'-C3'   | 7.37  | 131.25      | 120.20   |
| 53  | n     | 108  | VAL  | O-C-N       | 7.36  | 125.30      | 120.07   |
| 40  | a     | 2602 | A    | C4'-C3'-O3' | 7.29  | 120.33      | 109.40   |
| 40  | a     | 783  | A    | C4'-C3'-O3' | 7.27  | 123.90      | 113.00   |
| 20  | G     | 47   | VAL  | O-C-N       | 7.23  | 125.05      | 120.42   |
| 10  | B     | 29   | G    | N9-C1'-C2'  | -7.16 | 101.26      | 112.00   |
| 17  | D     | 1497 | G    | C1'-C2'-O2' | -7.14 | 97.69       | 108.40   |
| 17  | D     | 196  | A    | P-O3'-C3'   | 7.14  | 130.91      | 120.20   |
| 40  | a     | 2162 | G    | C4'-C3'-O3' | 7.12  | 120.08      | 109.40   |
| 40  | a     | 896  | A    | C4'-C3'-O3' | 7.04  | 119.96      | 109.40   |
| 40  | a     | 2225 | A    | C4'-C3'-O3' | 7.00  | 119.89      | 109.40   |
| 40  | a     | 1379 | U    | C2'-C3'-O3' | 6.98  | 124.17      | 113.70   |
| 26  | M     | 27   | VAL  | N-CA-CB     | 6.97  | 118.70      | 110.55   |
| 40  | a     | 2244 | U    | C4'-C3'-O3' | 6.90  | 123.34      | 113.00   |
| 21  | H     | 140  | PRO  | N-CA-CB     | 6.86  | 110.45      | 103.25   |
| 21  | H     | 340  | ARG  | CA-C-N      | -6.81 | 112.54      | 123.23   |
| 21  | H     | 340  | ARG  | C-N-CA      | -6.81 | 112.54      | 123.23   |
| 40  | a     | 2252 | G    | C4'-C3'-O3' | 6.78  | 123.18      | 113.00   |
| 53  | n     | 71   | ARG  | CA-C-N      | 6.76  | 134.00      | 122.37   |
| 53  | n     | 71   | ARG  | C-N-CA      | 6.76  | 134.00      | 122.37   |
| 40  | a     | 2243 | U    | C4'-C3'-O3' | 6.67  | 123.01      | 113.00   |
| 17  | D     | 517  | G    | C5'-C4'-C3' | 6.64  | 125.17      | 115.20   |
| 21  | H     | 170  | ARG  | N-CA-C      | 6.64  | 119.61      | 110.24   |
| 21  | H     | 87   | GLU  | N-CA-C      | -6.60 | 104.09      | 111.28   |
| 21  | H     | 303  | LEU  | N-CA-C      | 6.58  | 121.15      | 112.13   |
| 40  | a     | 2189 | U    | C1'-C2'-O2' | -6.58 | 101.92      | 111.80   |
| 21  | H     | 132  | PRO  | N-CA-CB     | 6.55  | 110.25      | 103.38   |
| 40  | a     | 2167 | U    | P-O3'-C3'   | 6.53  | 130.00      | 120.20   |
| 17  | D     | 526  | C    | C4'-C3'-O3' | 6.53  | 122.80      | 113.00   |
| 53  | n     | 127  | ASN  | CB-CA-C     | 6.53  | 121.67      | 110.77   |
| 21  | H     | 155  | LYS  | N-CA-C      | -6.52 | 98.28       | 108.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 40  | a     | 894  | U    | C2'-C3'-O3' | 6.52  | 119.27      | 109.50   |
| 21  | H     | 112  | ILE  | N-CA-C      | 6.51  | 117.07      | 106.72   |
| 28  | O     | 72   | ILE  | N-CA-C      | -6.51 | 105.36      | 111.48   |
| 57  | r     | 61   | VAL  | N-CA-CB     | 6.49  | 118.14      | 110.55   |
| 17  | D     | 526  | C    | N1-C1'-C2'  | -6.48 | 102.28      | 112.00   |
| 54  | o     | 13   | ARG  | N-CA-C      | 6.47  | 121.01      | 113.18   |
| 17  | D     | 1340 | A    | C1'-C2'-O2' | 6.47  | 118.10      | 108.40   |
| 53  | n     | 127  | ASN  | CA-CB-CG    | -6.43 | 106.17      | 112.60   |
| 40  | a     | 754  | U    | N1-C1'-C2'  | 6.40  | 121.61      | 112.00   |
| 17  | D     | 69   | G    | C4'-C3'-O3' | -6.35 | 103.47      | 113.00   |
| 12  | AB    | 122  | PRO  | N-CA-CB     | 6.33  | 109.89      | 103.25   |
| 17  | D     | 1208 | C    | N1-C1'-C2'  | -6.28 | 102.58      | 112.00   |
| 16  | C     | 33   | ILE  | CA-C-O      | -6.27 | 114.90      | 121.93   |
| 21  | H     | 153  | GLU  | N-CA-C      | -6.26 | 97.47       | 110.80   |
| 40  | a     | 2434 | A    | P-O3'-C3'   | 6.26  | 129.59      | 120.20   |
| 8   | 7     | 11   | U    | C4'-C3'-O3' | 6.23  | 118.74      | 109.40   |
| 10  | B     | 28   | C    | O3'-P-O5'   | -6.21 | 94.69       | 104.00   |
| 40  | a     | 2425 | A    | C4'-C3'-O3' | 6.20  | 118.70      | 109.40   |
| 21  | H     | 113  | ASN  | N-CA-C      | 6.16  | 118.08      | 111.36   |
| 17  | D     | 1206 | G    | N9-C1'-C2'  | -6.16 | 102.77      | 112.00   |
| 40  | a     | 271  | G    | C4'-C3'-O3' | 6.05  | 118.48      | 109.40   |
| 17  | D     | 1516 | G    | OP1-P-O3'   | -6.05 | 89.85       | 108.00   |
| 40  | a     | 2210 | U    | C4'-C3'-O3' | 6.00  | 118.39      | 109.40   |
| 17  | D     | 1408 | A    | C4'-C3'-O3' | 5.99  | 121.99      | 113.00   |
| 17  | D     | 550  | G    | C3'-C2'-O2' | 5.99  | 119.68      | 110.70   |
| 40  | a     | 2820 | A    | C4'-C3'-O3' | -5.98 | 104.03      | 113.00   |
| 40  | a     | 1913 | A    | C2'-C3'-O3' | 5.97  | 118.46      | 109.50   |
| 26  | M     | 92   | ARG  | CA-C-N      | 5.90  | 125.38      | 119.24   |
| 26  | M     | 92   | ARG  | C-N-CA      | 5.90  | 125.38      | 119.24   |
| 40  | a     | 2308 | G    | C2'-C3'-O3' | -5.88 | 104.89      | 113.70   |
| 51  | l     | 108  | ILE  | N-CA-CB     | 5.86  | 118.51      | 110.54   |
| 21  | H     | 109  | THR  | N-CA-C      | -5.86 | 99.11       | 109.06   |
| 40  | a     | 2756 | U    | C4'-C3'-O3' | 5.83  | 118.15      | 109.40   |
| 21  | H     | 150  | LYS  | N-CA-C      | 5.83  | 118.22      | 110.53   |
| 53  | n     | 72   | LYS  | N-CA-C      | -5.82 | 99.17       | 109.06   |
| 21  | H     | 75   | VAL  | N-CA-C      | 5.81  | 116.48      | 108.12   |
| 37  | X     | 26   | GLY  | N-CA-C      | -5.80 | 104.36      | 112.13   |
| 40  | a     | 1905 | C    | P-O3'-C3'   | 5.79  | 128.89      | 120.20   |
| 10  | B     | 29   | G    | O5'-C5'-C4' | -5.78 | 102.83      | 111.50   |
| 17  | D     | 1275 | A    | P-O3'-C3'   | 5.78  | 128.87      | 120.20   |
| 40  | a     | 70   | G    | C4'-C3'-O3' | 5.76  | 118.03      | 109.40   |
| 14  | AE    | 853  | THR  | CA-C-N      | 5.75  | 131.02      | 122.74   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | AE    | 853  | THR  | C-N-CA      | 5.75  | 131.02      | 122.74   |
| 10  | A     | 48   | C    | N1-C1'-C2'  | 5.72  | 120.59      | 112.00   |
| 10  | B     | 48   | C    | N1-C1'-C2'  | 5.72  | 120.59      | 112.00   |
| 17  | D     | 1406 | U    | N1-C1'-C2'  | -5.71 | 103.43      | 112.00   |
| 17  | D     | 1490 | U    | P-O3'-C3'   | 5.71  | 128.77      | 120.20   |
| 17  | D     | 1492 | A    | P-O3'-C3'   | 5.71  | 128.76      | 120.20   |
| 17  | D     | 976  | G    | C4'-C3'-O3' | -5.70 | 104.45      | 113.00   |
| 40  | a     | 2168 | G    | C4'-C3'-O3' | -5.69 | 104.47      | 113.00   |
| 40  | a     | 1757 | A    | C4'-C3'-O3' | -5.68 | 104.48      | 113.00   |
| 17  | D     | 1340 | A    | C5'-C4'-C3' | 5.67  | 124.50      | 116.00   |
| 40  | a     | 2017 | U    | C2'-C3'-O3' | -5.62 | 105.27      | 113.70   |
| 21  | H     | 114  | GLY  | N-CA-C      | 5.60  | 121.22      | 111.14   |
| 17  | D     | 780  | A    | C4'-C3'-O3' | -5.54 | 104.69      | 113.00   |
| 40  | a     | 2447 | G    | C2'-C3'-O3' | -5.52 | 101.21      | 109.50   |
| 40  | a     | 1568 | G    | C4'-C3'-O3' | -5.52 | 104.73      | 113.00   |
| 40  | a     | 2731 | G    | C4'-C3'-O3' | -5.51 | 104.74      | 113.00   |
| 14  | AE    | 1184 | ASP  | N-CA-C      | 5.43  | 121.81      | 109.81   |
| 40  | a     | 2572 | A    | C4'-C3'-O3' | -5.40 | 101.30      | 109.40   |
| 17  | D     | 864  | A    | N9-C1'-C2'  | 5.38  | 120.08      | 112.00   |
| 17  | D     | 1499 | A    | C4'-C3'-O3' | 5.38  | 121.07      | 113.00   |
| 40  | a     | 2068 | U    | C4'-C3'-O3' | -5.37 | 104.94      | 113.00   |
| 40  | a     | 944  | C    | C4'-C3'-O3' | -5.37 | 104.95      | 113.00   |
| 17  | D     | 1145 | A    | C4'-C3'-O3' | -5.36 | 104.95      | 113.00   |
| 40  | a     | 2481 | G    | C4'-C3'-O3' | -5.36 | 104.95      | 113.00   |
| 10  | B     | 35   | A    | P-O3'-C3'   | 5.35  | 128.23      | 120.20   |
| 17  | D     | 517  | G    | C4'-C3'-O3' | -5.35 | 101.38      | 109.40   |
| 40  | a     | 375  | G    | C2'-C3'-O3' | 5.32  | 121.68      | 113.70   |
| 46  | g     | 5    | ILE  | N-CA-C      | 5.32  | 117.70      | 111.05   |
| 40  | a     | 1270 | C    | C2'-C3'-O3' | -5.32 | 105.73      | 113.70   |
| 40  | a     | 2231 | U    | C1'-C2'-O2' | 5.31  | 116.36      | 108.40   |
| 17  | D     | 145  | G    | P-O3'-C3'   | 5.29  | 128.13      | 120.20   |
| 40  | a     | 2020 | A    | C4'-C3'-O3' | -5.29 | 105.07      | 113.00   |
| 37  | X     | 102  | THR  | CA-C-O      | -5.27 | 114.85      | 121.02   |
| 40  | a     | 2529 | G    | C4'-C3'-O3' | -5.26 | 105.11      | 113.00   |
| 17  | D     | 1395 | C    | P-O3'-C3'   | 5.25  | 128.07      | 120.20   |
| 8   | 7     | -11  | U    | C2'-C3'-O3' | 5.22  | 117.33      | 109.50   |
| 10  | B     | 60   | U    | C2'-C3'-O3' | 5.18  | 117.27      | 109.50   |
| 40  | a     | 423  | A    | C2'-C3'-O3' | -5.18 | 105.93      | 113.70   |
| 40  | a     | 2245 | U    | N1-C1'-C2'  | -5.17 | 104.24      | 112.00   |
| 38  | Y     | 5    | GLN  | O-C-N       | 5.17  | 124.65      | 120.83   |
| 10  | A     | 60   | U    | C2'-C3'-O3' | 5.17  | 117.25      | 109.50   |
| 21  | H     | 128  | ARG  | CA-C-N      | -5.16 | 114.14      | 122.81   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | H     | 128  | ARG  | C-N-CA      | -5.16 | 114.14      | 122.81   |
| 60  | u     | 101  | ILE  | N-CA-C      | 5.16  | 116.45      | 112.12   |
| 40  | a     | 1834 | U    | C4'-C3'-O3' | -5.15 | 105.27      | 113.00   |
| 40  | a     | 528  | A    | C4'-C3'-O3' | -5.13 | 105.30      | 113.00   |
| 17  | D     | 1335 | U    | C4'-C3'-O3' | -5.13 | 105.30      | 113.00   |
| 21  | H     | 154  | PHE  | N-CA-C      | -5.12 | 100.35      | 109.06   |
| 40  | a     | 479  | A    | C4'-C3'-O3' | 5.10  | 117.05      | 109.40   |
| 40  | a     | 328  | U    | C4'-C3'-O3' | -5.09 | 105.36      | 113.00   |
| 29  | P     | 25   | ILE  | N-CA-CB     | 5.09  | 117.46      | 110.54   |
| 14  | AE    | 709  | ARG  | CA-C-N      | 5.09  | 135.46      | 126.45   |
| 14  | AE    | 709  | ARG  | C-N-CA      | 5.09  | 135.46      | 126.45   |
| 40  | a     | 126  | A    | C4'-C3'-O3' | -5.09 | 105.37      | 113.00   |
| 16  | C     | 35   | GLU  | N-CA-C      | -5.07 | 105.94      | 111.82   |
| 40  | a     | 1864 | U    | C4'-C3'-O3' | -5.07 | 105.40      | 113.00   |
| 9   | 9     | 115  | GLY  | CA-C-O      | -5.05 | 118.19      | 122.29   |
| 40  | a     | 2193 | G    | C2'-C3'-O3' | 5.05  | 121.28      | 113.70   |
| 58  | s     | 28   | LEU  | CA-C-N      | 5.04  | 127.00      | 120.44   |
| 58  | s     | 28   | LEU  | C-N-CA      | 5.04  | 127.00      | 120.44   |
| 40  | a     | 614  | A    | C2'-C3'-O3' | 5.04  | 117.06      | 109.50   |
| 10  | B     | 19   | G    | N9-C1'-C2'  | 5.03  | 119.55      | 112.00   |
| 21  | H     | 108  | VAL  | N-CA-C      | -5.03 | 98.88       | 109.34   |
| 17  | D     | 70   | U    | C2'-C3'-O3' | 5.01  | 117.02      | 109.50   |

There are no chirality outliers.

All (16) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 10  | A     | 19   | G    | Sidechain |
| 10  | A     | 7    | G    | Sidechain |
| 11  | AA    | 910  | ALA  | Peptide   |
| 12  | AB    | 135  | ARG  | Sidechain |
| 13  | AC    | 192  | VAL  | Peptide   |
| 13  | AD    | 20   | SER  | Peptide   |
| 14  | AE    | 1326 | GLN  | Peptide   |
| 14  | AE    | 1344 | LEU  | Peptide   |
| 14  | AE    | 313  | GLY  | Peptide   |
| 14  | AE    | 416  | ILE  | Peptide   |
| 10  | B     | 19   | G    | Sidechain |
| 10  | B     | 7    | G    | Sidechain |
| 21  | H     | 274  | TYR  | Peptide   |
| 21  | H     | 81   | GLU  | Peptide   |
| 21  | H     | 82   | THR  | Peptide   |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 37  | X     | 100 | GLN  | Mainchain |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 816   | 839      | 839      | 8       | 0            |
| 2   | 1     | 857   | 922      | 922      | 14      | 0            |
| 3   | 2     | 746   | 811      | 811      | 6       | 0            |
| 4   | 3     | 788   | 844      | 844      | 11      | 0            |
| 5   | 4     | 753   | 780      | 780      | 0       | 0            |
| 6   | 5     | 472   | 260      | 260      | 17      | 0            |
| 7   | 6     | 542   | 305      | 306      | 28      | 0            |
| 8   | 7     | 707   | 97       | 351      | 108     | 0            |
| 9   | 9     | 1117  | 0        | 1153     | 165     | 0            |
| 10  | A     | 1620  | 826      | 826      | 174     | 0            |
| 10  | B     | 1620  | 813      | 827      | 141     | 0            |
| 11  | AA    | 10567 | 0        | 10584    | 159     | 0            |
| 12  | AB    | 1392  | 0        | 1373     | 259     | 0            |
| 13  | AC    | 1698  | 0        | 1718     | 13      | 0            |
| 13  | AD    | 1677  | 0        | 1713     | 30      | 0            |
| 14  | AE    | 10404 | 0        | 10622    | 209     | 0            |
| 15  | AF    | 650   | 0        | 658      | 10      | 0            |
| 16  | C     | 544   | 559      | 560      | 24      | 0            |
| 17  | D     | 32703 | 16423    | 16459    | 218     | 0            |
| 18  | E     | 669   | 719      | 719      | 4       | 0            |
| 19  | F     | 589   | 629      | 629      | 8       | 0            |
| 20  | G     | 1760  | 1785     | 1785     | 46      | 0            |
| 21  | H     | 1730  | 1454     | 1454     | 214     | 0            |
| 22  | I     | 1636  | 1710     | 1710     | 9       | 0            |
| 23  | J     | 1643  | 1707     | 1707     | 15      | 0            |
| 24  | K     | 1152  | 1196     | 1196     | 22      | 0            |
| 25  | L     | 848   | 846      | 846      | 4       | 0            |
| 26  | M     | 1181  | 1235     | 1235     | 34      | 0            |
| 27  | N     | 979   | 1031     | 1031     | 6       | 0            |
| 28  | O     | 1022  | 1070     | 1070     | 12      | 0            |
| 29  | P     | 790   | 831      | 831      | 123     | 0            |
| 30  | Q     | 877   | 887      | 887      | 4       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 31  | R     | 939    | 1001     | 1001     | 7       | 0            |
| 32  | S     | 805    | 844      | 844      | 4       | 0            |
| 33  | T     | 714    | 734      | 734      | 8       | 0            |
| 34  | U     | 649    | 666      | 666      | 3       | 0            |
| 35  | V     | 648    | 691      | 691      | 5       | 0            |
| 36  | W     | 663    | 688      | 688      | 3       | 0            |
| 37  | X     | 900    | 964      | 964      | 57      | 0            |
| 38  | Y     | 1032   | 0        | 1088     | 83      | 0            |
| 39  | Z     | 227    | 0        | 237      | 17      | 0            |
| 40  | a     | 61841  | 31077    | 31123    | 299     | 0            |
| 41  | b     | 582    | 599      | 599      | 2       | 0            |
| 42  | c     | 625    | 652      | 652      | 4       | 0            |
| 43  | d     | 2569   | 1301     | 1301     | 4       | 0            |
| 44  | e     | 501    | 531      | 531      | 4       | 0            |
| 45  | f     | 448    | 488      | 488      | 5       | 0            |
| 46  | g     | 522    | 520      | 520      | 11      | 0            |
| 47  | h     | 2082   | 2154     | 2154     | 17      | 0            |
| 48  | i     | 444    | 459      | 458      | 5       | 0            |
| 49  | j     | 1565   | 1617     | 1616     | 15      | 0            |
| 50  | k     | 426    | 464      | 464      | 0       | 0            |
| 51  | l     | 1552   | 1619     | 1619     | 13      | 0            |
| 52  | m     | 377    | 418      | 418      | 10      | 0            |
| 53  | n     | 1410   | 1443     | 1444     | 27      | 0            |
| 54  | o     | 504    | 572      | 572      | 3       | 0            |
| 55  | p     | 1313   | 1358     | 1358     | 7       | 0            |
| 56  | q     | 302    | 343      | 343      | 1       | 0            |
| 57  | r     | 1111   | 1148     | 1148     | 6       | 0            |
| 58  | s     | 1129   | 1162     | 1162     | 14      | 0            |
| 59  | t     | 946    | 1023     | 1023     | 12      | 0            |
| 60  | u     | 1053   | 1129     | 1129     | 7       | 0            |
| 61  | v     | 1074   | 1157     | 1157     | 5       | 0            |
| 62  | w     | 951    | 994      | 994      | 8       | 0            |
| 63  | x     | 892    | 923      | 923      | 8       | 0            |
| 64  | y     | 917    | 962      | 962      | 4       | 0            |
| 65  | z     | 947    | 1020     | 1019     | 13      | 0            |
| 66  | AE    | 1      | 0        | 0        | 0       | 0            |
| 67  | AE    | 2      | 0        | 0        | 3       | 0            |
| All | All   | 177212 | 99300    | 128796   | 2259    | 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 7.

All (2259) 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) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:AE:79:LYS:HA    | 14:AE:81:ARG:CZ   | 1.26                     | 1.65              |
| 16:C:12:ARG:HG3    | 21:H:264:GLU:CB   | 1.30                     | 1.61              |
| 12:AB:164:ILE:HB   | 29:P:88:MET:CG    | 1.26                     | 1.58              |
| 21:H:131:LEU:CB    | 21:H:167:VAL:CA   | 1.78                     | 1.57              |
| 12:AB:164:ILE:CD1  | 12:AB:168:ALA:HB3 | 1.32                     | 1.53              |
| 12:AB:171:VAL:CG2  | 29:P:102:LEU:HB3  | 1.35                     | 1.53              |
| 21:H:131:LEU:CB    | 21:H:167:VAL:HA   | 1.03                     | 1.49              |
| 14:AE:72:CYS:SG    | 67:AE:1502:ZN:ZN  | 1.03                     | 1.45              |
| 12:AB:164:ILE:HB   | 29:P:88:MET:SD    | 1.55                     | 1.45              |
| 14:AE:79:LYS:HA    | 14:AE:81:ARG:NH1  | 1.20                     | 1.45              |
| 9:9:130:PRO:N      | 9:9:130:PRO:CA    | 1.70                     | 1.42              |
| 9:9:31:ARG:NE      | 40:a:1054:A:H5'   | 1.31                     | 1.36              |
| 21:H:71:ALA:C      | 21:H:72:LEU:HD12  | 1.49                     | 1.36              |
| 12:AB:133:MET:CG   | 12:AB:146:GLY:O   | 1.74                     | 1.35              |
| 9:9:57:ASN:OD1     | 9:9:62:ARG:CG     | 1.75                     | 1.34              |
| 17:D:1358:U:O4     | 17:D:1363:A:N1    | 1.60                     | 1.34              |
| 21:H:118:GLY:O     | 21:H:133:GLY:CA   | 1.74                     | 1.34              |
| 12:AB:45:PRO:N     | 12:AB:45:PRO:CA   | 1.70                     | 1.34              |
| 14:AE:79:LYS:CA    | 14:AE:81:ARG:CZ   | 2.06                     | 1.33              |
| 14:AE:79:LYS:CA    | 14:AE:81:ARG:NH1  | 1.90                     | 1.33              |
| 40:a:1839:G:H1'    | 40:a:1927:A:C8    | 1.62                     | 1.33              |
| 12:AB:141:PHE:CE1  | 29:P:84:VAL:HG11  | 1.64                     | 1.31              |
| 14:AE:47:ARG:HE    | 29:P:81:GLU:CD    | 1.39                     | 1.31              |
| 12:AB:146:GLY:C    | 12:AB:163:SER:OG  | 1.75                     | 1.30              |
| 40:a:1021:A:N1     | 40:a:1141:U:O4    | 1.63                     | 1.30              |
| 12:AB:164:ILE:HD11 | 12:AB:168:ALA:CB  | 1.61                     | 1.30              |
| 12:AB:133:MET:HG2  | 12:AB:146:GLY:O   | 1.26                     | 1.29              |
| 7:6:5:DT:OP1       | 14:AE:1172:LYS:NZ | 1.68                     | 1.27              |
| 12:AB:164:ILE:CD1  | 12:AB:168:ALA:CB  | 2.12                     | 1.27              |
| 12:AB:44:VAL:CB    | 12:AB:45:PRO:HD2  | 1.65                     | 1.27              |
| 9:9:31:ARG:CZ      | 40:a:1054:A:H5'   | 1.63                     | 1.26              |
| 12:AB:147:VAL:N    | 12:AB:163:SER:OG  | 1.69                     | 1.26              |
| 17:D:1308:U:H2'    | 37:X:98:ARG:NH2   | 1.48                     | 1.26              |
| 12:AB:147:VAL:HG23 | 12:AB:163:SER:OG  | 1.35                     | 1.26              |
| 16:C:12:ARG:CG     | 21:H:264:GLU:CB   | 2.15                     | 1.25              |
| 17:D:948:C:OP2     | 37:X:105:ASN:OD1  | 1.53                     | 1.25              |
| 17:D:1227:A:OP2    | 37:X:110:LYS:HE3  | 1.35                     | 1.25              |
| 12:AB:164:ILE:CB   | 29:P:88:MET:SD    | 2.22                     | 1.25              |
| 21:H:118:GLY:O     | 21:H:133:GLY:HA3  | 1.27                     | 1.24              |
| 10:A:32:C:O4'      | 26:M:144:MET:HE1  | 1.09                     | 1.24              |
| 17:D:1308:U:H3'    | 37:X:98:ARG:CZ    | 1.43                     | 1.23              |
| 10:A:18:G:N7       | 10:A:57:A:N6      | 1.87                     | 1.23              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 21:H:267:TRP:CZ2   | 21:H:340:ARG:HG2    | 1.75                     | 1.22              |
| 17:D:563:A:N1      | 17:D:884:U:O4       | 1.73                     | 1.22              |
| 10:B:18:G:N7       | 10:B:57:A:N6        | 1.87                     | 1.21              |
| 17:D:1308:U:C2'    | 37:X:98:ARG:NH2     | 2.03                     | 1.21              |
| 12:AB:171:VAL:HG23 | 29:P:102:LEU:CB     | 1.70                     | 1.21              |
| 12:AB:140:PRO:CG   | 29:P:79:PRO:HB2     | 1.69                     | 1.20              |
| 12:AB:164:ILE:CB   | 29:P:88:MET:CG      | 2.19                     | 1.20              |
| 9:9:88:HIS:HB3     | 9:9:89:PRO:CD       | 1.70                     | 1.20              |
| 9:9:142:THR:HG21   | 39:Z:7:ILE:HG12     | 1.21                     | 1.17              |
| 9:9:31:ARG:NE      | 40:a:1054:A:C5'     | 2.07                     | 1.16              |
| 8:7:11:U:O2        | 11:AA:1253:LEU:HD12 | 1.43                     | 1.15              |
| 6:5:100:DA:H5'     | 14:AE:278:ARG:NH1   | 1.62                     | 1.14              |
| 12:AB:133:MET:HG3  | 12:AB:146:GLY:C     | 1.71                     | 1.13              |
| 14:AE:47:ARG:NE    | 29:P:81:GLU:CD      | 2.06                     | 1.13              |
| 21:H:135:LEU:CB    | 21:H:167:VAL:CB     | 2.27                     | 1.13              |
| 20:G:19:GLN:CD     | 21:H:76:GLU:CB      | 2.19                     | 1.13              |
| 10:A:32:C:O4'      | 26:M:144:MET:CE     | 1.97                     | 1.12              |
| 10:B:70:G:H2'      | 10:B:71:C:H5''      | 1.23                     | 1.12              |
| 16:C:44:ILE:HD13   | 21:H:339:ARG:CG     | 1.78                     | 1.12              |
| 20:G:19:GLN:CD     | 21:H:76:GLU:HB3     | 1.67                     | 1.12              |
| 12:AB:171:VAL:CG2  | 29:P:102:LEU:CB     | 2.24                     | 1.12              |
| 17:D:1329:A:OP1    | 37:X:28:THR:HB      | 1.47                     | 1.12              |
| 21:H:267:TRP:CE2   | 21:H:340:ARG:HG2    | 1.84                     | 1.11              |
| 16:C:44:ILE:HD13   | 21:H:339:ARG:HG2    | 1.18                     | 1.11              |
| 12:AB:147:VAL:CG2  | 12:AB:163:SER:OG    | 1.98                     | 1.11              |
| 14:AE:79:LYS:HA    | 14:AE:81:ARG:NH2    | 1.66                     | 1.11              |
| 12:AB:133:MET:HG3  | 12:AB:163:SER:OG    | 1.49                     | 1.10              |
| 12:AB:44:VAL:HB    | 12:AB:45:PRO:CD     | 1.80                     | 1.10              |
| 14:AE:47:ARG:NE    | 29:P:81:GLU:OE1     | 1.83                     | 1.10              |
| 21:H:267:TRP:CH2   | 21:H:340:ARG:HG2    | 1.87                     | 1.10              |
| 9:9:88:HIS:CB      | 9:9:89:PRO:HD3      | 1.82                     | 1.09              |
| 10:A:70:G:H2'      | 10:A:71:C:H5''      | 1.22                     | 1.09              |
| 9:9:129:LEU:N      | 9:9:130:PRO:HD3     | 1.66                     | 1.09              |
| 12:AB:141:PHE:CD1  | 29:P:84:VAL:HG11    | 1.86                     | 1.09              |
| 17:D:1308:U:C3'    | 37:X:98:ARG:NH2     | 2.16                     | 1.09              |
| 9:9:50:VAL:HG22    | 38:Y:119:ALA:CB     | 1.82                     | 1.08              |
| 11:AA:887:VAL:HB   | 11:AA:913:VAL:HG21  | 1.28                     | 1.08              |
| 23:J:162:ALA:HA    | 23:J:165:ARG:CZ     | 1.83                     | 1.08              |
| 21:H:71:ALA:O      | 21:H:72:LEU:HD12    | 1.54                     | 1.08              |
| 40:a:1839:G:C8     | 40:a:1927:A:H1'     | 1.87                     | 1.08              |
| 17:D:1308:U:C2'    | 37:X:98:ARG:HH21    | 1.63                     | 1.08              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:H:119:GLY:HA2   | 21:H:133:GLY:HA2   | 1.14                     | 1.08              |
| 9:9:57:ASN:OD1     | 9:9:62:ARG:HG3     | 1.44                     | 1.08              |
| 12:AB:164:ILE:HG13 | 29:P:88:MET:CA     | 1.84                     | 1.08              |
| 12:AB:164:ILE:HG13 | 29:P:88:MET:HA     | 1.23                     | 1.08              |
| 17:D:1308:U:C3'    | 37:X:98:ARG:CZ     | 2.31                     | 1.07              |
| 11:AA:845:LEU:CD2  | 11:AA:890:LYS:O    | 2.02                     | 1.07              |
| 12:AB:170:PRO:HD2  | 29:P:100:ILE:HB    | 1.23                     | 1.07              |
| 12:AB:168:ALA:HB2  | 29:P:88:MET:HA     | 1.29                     | 1.06              |
| 8:7:-18:G:H5''     | 17:D:1500:A:N6     | 1.69                     | 1.06              |
| 20:G:19:GLN:HG3    | 21:H:75:VAL:HG22   | 1.38                     | 1.05              |
| 11:AA:887:VAL:HB   | 11:AA:913:VAL:CG2  | 1.85                     | 1.05              |
| 12:AB:133:MET:CG   | 12:AB:146:GLY:C    | 2.25                     | 1.05              |
| 12:AB:146:GLY:CA   | 12:AB:162:VAL:C    | 2.28                     | 1.05              |
| 20:G:19:GLN:CG     | 21:H:75:VAL:HG22   | 1.84                     | 1.05              |
| 21:H:162:LYS:CB    | 21:H:298:GLU:CD    | 2.30                     | 1.04              |
| 17:D:1227:A:OP2    | 37:X:110:LYS:CE    | 2.06                     | 1.04              |
| 10:A:18:G:N2       | 10:A:55:U:O2       | 1.90                     | 1.04              |
| 10:B:56:C:O4'      | 53:n:80:ARG:NH2    | 1.91                     | 1.04              |
| 21:H:19:ARG:O      | 21:H:72:LEU:HB2    | 1.58                     | 1.03              |
| 12:AB:133:MET:SD   | 12:AB:163:SER:HB2  | 1.97                     | 1.03              |
| 6:5:99:DT:OP1      | 12:AB:63:LYS:HE3   | 1.56                     | 1.03              |
| 12:AB:133:MET:HG3  | 12:AB:163:SER:HG   | 0.86                     | 1.03              |
| 10:B:18:G:N2       | 10:B:55:U:O2       | 1.90                     | 1.03              |
| 8:7:-10:U:O2'      | 24:K:33:PHE:CE1    | 2.11                     | 1.03              |
| 10:B:70:G:C2'      | 10:B:71:C:H5''     | 1.89                     | 1.02              |
| 17:D:1329:A:OP1    | 37:X:28:THR:CB     | 2.07                     | 1.02              |
| 8:7:14:U:H4'       | 14:AE:322:ARG:CD   | 1.88                     | 1.02              |
| 12:AB:164:ILE:HD12 | 12:AB:168:ALA:HB3  | 1.41                     | 1.02              |
| 10:B:56:C:H2'      | 10:B:57:A:H5''     | 1.39                     | 1.02              |
| 12:AB:146:GLY:HA2  | 12:AB:163:SER:CB   | 1.89                     | 1.02              |
| 12:AB:164:ILE:HB   | 29:P:88:MET:CB     | 1.88                     | 1.02              |
| 12:AB:141:PHE:CE1  | 29:P:84:VAL:CG1    | 2.42                     | 1.02              |
| 12:AB:146:GLY:HA3  | 12:AB:162:VAL:C    | 1.85                     | 1.02              |
| 9:9:129:LEU:H      | 9:9:130:PRO:HD3    | 0.90                     | 1.01              |
| 10:A:70:G:C2'      | 10:A:71:C:H5''     | 1.89                     | 1.01              |
| 12:AB:164:ILE:HB   | 29:P:88:MET:HG3    | 1.36                     | 1.01              |
| 10:B:56:C:H5'      | 53:n:80:ARG:CZ     | 1.90                     | 1.01              |
| 8:7:12:G:C1'       | 14:AE:253:VAL:HG11 | 1.89                     | 1.01              |
| 20:G:38:VAL:CG2    | 21:H:75:VAL:HG21   | 1.90                     | 1.01              |
| 8:7:12:G:H1'       | 14:AE:253:VAL:HG11 | 1.41                     | 1.01              |
| 21:H:290:TYR:O     | 21:H:305:HIS:O     | 1.77                     | 1.01              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:9:93:ALA:O       | 9:9:129:LEU:HD12   | 1.60                     | 1.00              |
| 10:A:56:C:H2'      | 10:A:57:A:H5''     | 1.38                     | 1.00              |
| 17:D:13:U:N3       | 17:D:915:A:C6      | 2.29                     | 1.00              |
| 17:D:13:U:O4       | 17:D:20:U:O4       | 1.79                     | 1.00              |
| 12:AB:65:PHE:CE2   | 12:AB:68:TYR:O     | 2.15                     | 1.00              |
| 10:A:32:C:C4'      | 26:M:144:MET:HE1   | 1.93                     | 0.99              |
| 40:a:2297:A:N1     | 40:a:2321:U:C4     | 2.29                     | 0.99              |
| 12:AB:140:PRO:HG3  | 29:P:79:PRO:HB2    | 1.40                     | 0.98              |
| 12:AB:146:GLY:CA   | 12:AB:163:SER:N    | 2.25                     | 0.98              |
| 21:H:131:LEU:CB    | 21:H:167:VAL:CB    | 2.40                     | 0.98              |
| 17:D:1308:U:H2'    | 37:X:98:ARG:HH21   | 1.06                     | 0.98              |
| 40:a:1839:G:O4'    | 40:a:1927:A:O4'    | 1.82                     | 0.98              |
| 9:9:31:ARG:CD      | 40:a:1054:A:H5'    | 1.94                     | 0.98              |
| 10:A:32:C:O2'      | 26:M:86:GLN:CG     | 2.12                     | 0.98              |
| 12:AB:146:GLY:HA2  | 12:AB:163:SER:N    | 1.77                     | 0.98              |
| 40:a:1839:G:C1'    | 40:a:1927:A:C8     | 2.46                     | 0.98              |
| 9:9:129:LEU:H      | 9:9:130:PRO:CD     | 1.77                     | 0.97              |
| 17:D:1308:U:H3'    | 37:X:98:ARG:NH2    | 1.76                     | 0.97              |
| 21:H:119:GLY:CA    | 21:H:133:GLY:HA2   | 1.95                     | 0.97              |
| 8:7:-19:U:P        | 17:D:1505:G:H8     | 1.87                     | 0.97              |
| 20:G:38:VAL:HG22   | 21:H:75:VAL:HG21   | 1.44                     | 0.97              |
| 9:9:57:ASN:OD1     | 9:9:62:ARG:HG2     | 1.64                     | 0.96              |
| 12:AB:133:MET:HG3  | 12:AB:146:GLY:O    | 1.57                     | 0.96              |
| 9:9:88:HIS:CB      | 9:9:89:PRO:CD      | 2.41                     | 0.96              |
| 12:AB:147:VAL:HG23 | 12:AB:163:SER:CB   | 1.93                     | 0.96              |
| 9:9:142:THR:HG21   | 39:Z:7:ILE:CG1     | 1.95                     | 0.96              |
| 21:H:118:GLY:O     | 21:H:133:GLY:HA2   | 1.63                     | 0.96              |
| 11:AA:845:LEU:HD22 | 11:AA:890:LYS:O    | 1.66                     | 0.96              |
| 12:AB:65:PHE:HZ    | 12:AB:70:LEU:HD13  | 1.25                     | 0.96              |
| 8:7:14:U:H4'       | 14:AE:322:ARG:HD3  | 1.48                     | 0.96              |
| 12:AB:44:VAL:HB    | 12:AB:45:PRO:HD2   | 0.96                     | 0.95              |
| 12:AB:140:PRO:HG3  | 29:P:79:PRO:CB     | 1.95                     | 0.95              |
| 11:AA:887:VAL:CB   | 11:AA:913:VAL:HG21 | 1.96                     | 0.95              |
| 12:AB:145:ASN:O    | 12:AB:162:VAL:O    | 1.84                     | 0.95              |
| 7:6:15:DC:N4       | 7:6:16:DC:N4       | 2.15                     | 0.95              |
| 12:AB:164:ILE:HG13 | 12:AB:168:ALA:HB2  | 1.47                     | 0.95              |
| 12:AB:164:ILE:HG13 | 29:P:88:MET:CB     | 1.96                     | 0.95              |
| 40:a:1839:G:O4'    | 40:a:1927:A:C1'    | 2.15                     | 0.95              |
| 10:B:72:A:H2'      | 10:B:73:A:H5''     | 1.49                     | 0.94              |
| 40:a:67:U:N3       | 40:a:74:A:C6       | 2.35                     | 0.94              |
| 14:AE:85:CYS:HG    | 67:AE:1502:ZN:ZN   | 0.66                     | 0.94              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:A:72:A:H2'      | 10:A:73:A:H5''    | 1.49                     | 0.94              |
| 17:D:13:U:C4       | 17:D:915:A:N6     | 2.36                     | 0.94              |
| 12:AB:140:PRO:HG2  | 29:P:79:PRO:HB2   | 1.47                     | 0.94              |
| 12:AB:171:VAL:HG21 | 29:P:102:LEU:HB3  | 1.47                     | 0.94              |
| 12:AB:141:PHE:HE1  | 29:P:84:VAL:CG1   | 1.78                     | 0.94              |
| 12:AB:146:GLY:HA3  | 12:AB:162:VAL:CA  | 1.97                     | 0.94              |
| 17:D:13:U:N3       | 17:D:915:A:N6     | 2.16                     | 0.94              |
| 10:A:32:C:O2'      | 26:M:86:GLN:HG3   | 1.68                     | 0.93              |
| 12:AB:133:MET:CG   | 12:AB:163:SER:HG  | 1.80                     | 0.93              |
| 14:AE:79:LYS:HA    | 14:AE:81:ARG:HH12 | 1.32                     | 0.93              |
| 21:H:135:LEU:HA    | 21:H:157:ILE:CB   | 1.98                     | 0.93              |
| 11:AA:855:PRO:HG3  | 11:AA:912:ASP:O   | 1.69                     | 0.93              |
| 9:9:88:HIS:HB3     | 9:9:89:PRO:HD3    | 0.93                     | 0.92              |
| 10:B:75:C:OP1      | 40:a:2602:A:C8    | 2.23                     | 0.92              |
| 21:H:119:GLY:HA3   | 21:H:131:LEU:O    | 1.68                     | 0.92              |
| 14:AE:59:ALA:CB    | 14:AE:71:LEU:HD21 | 1.99                     | 0.92              |
| 12:AB:141:PHE:HE1  | 29:P:84:VAL:HG11  | 1.24                     | 0.92              |
| 17:D:13:U:C4       | 17:D:20:U:O4      | 2.23                     | 0.91              |
| 21:H:71:ALA:C      | 21:H:72:LEU:CD1   | 2.42                     | 0.91              |
| 7:6:5:DT:P         | 14:AE:1172:LYS:NZ | 2.43                     | 0.91              |
| 9:9:50:VAL:HG22    | 38:Y:119:ALA:HB1  | 1.50                     | 0.91              |
| 12:AB:19:GLU:OE2   | 12:AB:65:PHE:HD2  | 1.53                     | 0.91              |
| 40:a:1406:U:O2'    | 40:a:1407:G:C5'   | 2.19                     | 0.91              |
| 8:7:-17:U:O2'      | 17:D:1403:C:O2    | 1.87                     | 0.91              |
| 10:A:56:C:H1'      | 40:a:2112:G:C6    | 2.06                     | 0.91              |
| 8:7:-19:U:P        | 17:D:1505:G:C8    | 2.64                     | 0.91              |
| 10:A:68:C:H2'      | 10:A:69:C:H5''    | 1.51                     | 0.91              |
| 38:Y:104:GLN:HG2   | 38:Y:108:ILE:HD11 | 1.53                     | 0.90              |
| 9:9:93:ALA:O       | 9:9:129:LEU:CD1   | 2.19                     | 0.90              |
| 21:H:119:GLY:HA2   | 21:H:133:GLY:CA   | 2.01                     | 0.90              |
| 21:H:279:LYS:HA    | 21:H:331:MET:HB3  | 1.54                     | 0.90              |
| 40:a:2013:A:N6     | 40:a:2613:U:H3    | 1.68                     | 0.90              |
| 8:7:-18:G:C5'      | 17:D:1500:A:H62   | 1.85                     | 0.90              |
| 10:B:18:G:N2       | 10:B:58:A:N7      | 2.19                     | 0.90              |
| 14:AE:47:ARG:NE    | 29:P:81:GLU:OE2   | 2.04                     | 0.90              |
| 9:9:129:LEU:N      | 9:9:130:PRO:CD    | 2.34                     | 0.90              |
| 10:A:18:G:N2       | 10:A:58:A:N7      | 2.19                     | 0.90              |
| 12:AB:171:VAL:HG23 | 29:P:102:LEU:HB3  | 0.91                     | 0.90              |
| 10:B:68:C:H2'      | 10:B:69:C:H5''    | 1.50                     | 0.90              |
| 21:H:162:LYS:N     | 21:H:298:GLU:OE2  | 2.06                     | 0.89              |
| 12:AB:164:ILE:CG1  | 12:AB:168:ALA:CB  | 2.51                     | 0.89              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:Y:21:PRO:HB2   | 38:Y:22:PRO:HD3    | 1.54                     | 0.89              |
| 10:A:33:U:H5''    | 26:M:84:THR:HG21   | 1.55                     | 0.88              |
| 12:AB:164:ILE:HA  | 29:P:88:MET:SD     | 2.13                     | 0.88              |
| 9:9:142:THR:CG2   | 39:Z:7:ILE:HG12    | 2.02                     | 0.88              |
| 12:AB:44:VAL:CG1  | 12:AB:45:PRO:HD2   | 2.03                     | 0.88              |
| 12:AB:164:ILE:CG1 | 12:AB:168:ALA:HB2  | 2.04                     | 0.88              |
| 12:AB:146:GLY:HA2 | 12:AB:162:VAL:C    | 1.93                     | 0.87              |
| 12:AB:170:PRO:HG2 | 29:P:100:ILE:O     | 1.74                     | 0.87              |
| 40:a:2314:A:H1'   | 53:n:155:THR:HG21  | 1.54                     | 0.87              |
| 12:AB:145:ASN:O   | 12:AB:162:VAL:HG12 | 1.75                     | 0.87              |
| 14:AE:78:LEU:C    | 14:AE:81:ARG:HH11  | 1.79                     | 0.87              |
| 12:AB:65:PHE:CZ   | 12:AB:70:LEU:HD13  | 2.08                     | 0.87              |
| 20:G:18:HIS:HA    | 21:H:43:LYS:HD2    | 1.55                     | 0.87              |
| 9:9:31:ARG:CZ     | 40:a:1054:A:C5'    | 2.49                     | 0.87              |
| 12:AB:164:ILE:CA  | 29:P:88:MET:SD     | 2.63                     | 0.87              |
| 14:AE:59:ALA:CB   | 14:AE:71:LEU:CD2   | 2.51                     | 0.87              |
| 21:H:131:LEU:CB   | 21:H:167:VAL:N     | 2.37                     | 0.87              |
| 12:AB:164:ILE:CB  | 29:P:88:MET:HG3    | 1.97                     | 0.87              |
| 46:g:16:CYS:CB    | 46:g:37:CYS:HB3    | 2.05                     | 0.87              |
| 16:C:31:ASN:OD1   | 21:H:268:VAL:HG22  | 1.74                     | 0.87              |
| 21:H:348:GLN:N    | 21:H:348:GLN:OE1   | 2.08                     | 0.86              |
| 12:AB:44:VAL:CB   | 12:AB:45:PRO:CD    | 2.47                     | 0.86              |
| 9:9:50:VAL:CG2    | 38:Y:119:ALA:HB3   | 2.04                     | 0.86              |
| 23:J:162:ALA:HB2  | 23:J:165:ARG:NH2   | 1.90                     | 0.86              |
| 12:AB:144:PHE:CZ  | 29:P:81:GLU:O      | 2.29                     | 0.86              |
| 14:AE:79:LYS:N    | 14:AE:81:ARG:NH1   | 2.22                     | 0.86              |
| 40:a:783:A:N3     | 40:a:783:A:H2'     | 1.89                     | 0.86              |
| 10:A:16:C:O2      | 40:a:2181:U:H5'    | 1.76                     | 0.86              |
| 10:B:18:G:N7      | 10:B:57:A:C6       | 2.44                     | 0.86              |
| 38:Y:81:LYS:O     | 38:Y:81:LYS:HE3    | 1.75                     | 0.86              |
| 21:H:267:TRP:CZ3  | 21:H:340:ARG:HG2   | 2.11                     | 0.85              |
| 9:9:125:ARG:NH1   | 9:9:125:ARG:HA     | 1.92                     | 0.85              |
| 9:9:52:MET:C      | 9:9:52:MET:HE3     | 2.00                     | 0.85              |
| 23:J:61:VAL:HG21  | 23:J:200:ILE:HD11  | 1.57                     | 0.85              |
| 9:9:31:ARG:CD     | 40:a:1054:A:H4'    | 2.06                     | 0.85              |
| 40:a:67:U:N3      | 40:a:74:A:N6       | 2.25                     | 0.85              |
| 17:D:197:A:C6     | 17:D:221:C:H4'     | 2.11                     | 0.85              |
| 21:H:332:VAL:HG11 | 21:H:335:ILE:HG13  | 1.57                     | 0.85              |
| 38:Y:60:VAL:HG13  | 38:Y:66:PHE:HB3    | 1.58                     | 0.85              |
| 10:A:18:G:N7      | 10:A:57:A:C6       | 2.44                     | 0.85              |
| 12:AB:144:PHE:CE1 | 29:P:85:ASP:OD2    | 2.29                     | 0.85              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 16:C:12:ARG:HH22   | 21:H:268:VAL:CG2  | 1.90                     | 0.85              |
| 12:AB:164:ILE:HD11 | 12:AB:168:ALA:HB3 | 0.85                     | 0.84              |
| 20:G:16:PHE:HB3    | 21:H:43:LYS:HA    | 1.59                     | 0.84              |
| 21:H:135:LEU:CB    | 21:H:167:VAL:C    | 2.50                     | 0.84              |
| 40:a:2303:G:C2     | 40:a:2314:A:C2    | 2.66                     | 0.84              |
| 12:AB:164:ILE:CB   | 29:P:88:MET:HB2   | 2.08                     | 0.84              |
| 21:H:131:LEU:CB    | 21:H:166:VAL:O    | 2.26                     | 0.84              |
| 7:6:21:DA:N1       | 8:7:15:G:N2       | 2.26                     | 0.84              |
| 9:9:31:ARG:HH11    | 9:9:31:ARG:HG3    | 1.41                     | 0.84              |
| 21:H:267:TRP:CD2   | 21:H:340:ARG:HG2  | 2.11                     | 0.84              |
| 38:Y:20:SER:HB3    | 38:Y:21:PRO:HD3   | 1.59                     | 0.83              |
| 12:AB:146:GLY:HA2  | 12:AB:163:SER:HB2 | 1.57                     | 0.83              |
| 9:9:28:ALA:H       | 9:9:110:ALA:HA    | 1.44                     | 0.83              |
| 9:9:31:ARG:CD      | 40:a:1054:A:C4'   | 2.56                     | 0.83              |
| 12:AB:164:ILE:CG2  | 29:P:88:MET:SD    | 2.65                     | 0.83              |
| 14:AE:78:LEU:C     | 14:AE:81:ARG:NH1  | 2.24                     | 0.83              |
| 10:B:72:A:C2'      | 10:B:73:A:H5''    | 2.09                     | 0.83              |
| 4:3:34:VAL:HG13    | 4:3:67:VAL:HG22   | 1.58                     | 0.83              |
| 10:B:56:C:H5'      | 53:n:80:ARG:NE    | 1.93                     | 0.83              |
| 10:B:68:C:C2'      | 10:B:69:C:H5''    | 2.08                     | 0.83              |
| 8:7:-18:G:C5'      | 17:D:1500:A:N6    | 2.42                     | 0.83              |
| 7:6:18:DC:H42      | 8:7:17:G:H1       | 1.27                     | 0.83              |
| 12:AB:164:ILE:CB   | 29:P:88:MET:CB    | 2.52                     | 0.83              |
| 21:H:267:TRP:CH2   | 21:H:340:ARG:CG   | 2.60                     | 0.83              |
| 10:A:68:C:C2'      | 10:A:69:C:H5''    | 2.08                     | 0.83              |
| 12:AB:146:GLY:HA3  | 12:AB:162:VAL:HA  | 1.58                     | 0.83              |
| 10:A:72:A:C2'      | 10:A:73:A:H5''    | 2.09                     | 0.82              |
| 17:D:1227:A:H5'    | 37:X:110:LYS:NZ   | 1.94                     | 0.82              |
| 38:Y:102:ARG:HB3   | 38:Y:141:ASP:HA   | 1.61                     | 0.82              |
| 40:a:1019:U:H3     | 40:a:1142:A:H61   | 1.28                     | 0.82              |
| 8:7:-19:U:OP2      | 17:D:1505:G:C8    | 2.32                     | 0.82              |
| 9:9:62:ARG:HG2     | 9:9:62:ARG:HH21   | 1.44                     | 0.82              |
| 10:A:54:U:H3       | 10:A:58:A:N6      | 1.77                     | 0.82              |
| 40:a:1021:A:N6     | 40:a:1141:U:H3    | 1.77                     | 0.82              |
| 40:a:1839:G:C1'    | 40:a:1927:A:N9    | 2.43                     | 0.82              |
| 9:9:43:LYS:HD2     | 9:9:43:LYS:C      | 2.05                     | 0.82              |
| 12:AB:164:ILE:HG13 | 12:AB:168:ALA:CB  | 2.10                     | 0.82              |
| 40:a:1406:U:O2'    | 40:a:1407:G:H5''  | 1.79                     | 0.82              |
| 8:7:-19:U:OP1      | 17:D:1505:G:C8    | 2.32                     | 0.82              |
| 12:AB:158:LEU:HD21 | 12:AB:175:PHE:CE1 | 2.14                     | 0.82              |
| 9:9:57:ASN:OD1     | 9:9:62:ARG:CD     | 2.27                     | 0.81              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AB:144:PHE:CE2  | 29:P:81:GLU:HG3    | 2.15                     | 0.81              |
| 8:7:2:U:OP1        | 14:AE:77:ARG:NH2   | 2.13                     | 0.81              |
| 9:9:31:ARG:HD2     | 40:a:1054:A:H4'    | 1.62                     | 0.81              |
| 24:K:111:MET:HE2   | 24:K:125:ALA:HB1   | 1.59                     | 0.81              |
| 10:A:56:C:C2'      | 10:A:57:A:H5''     | 2.10                     | 0.81              |
| 21:H:155:LYS:CB    | 21:H:169:SER:CB    | 2.58                     | 0.81              |
| 8:7:-19:U:OP1      | 17:D:1505:G:H8     | 1.62                     | 0.81              |
| 16:C:12:ARG:CB     | 21:H:264:GLU:CB    | 2.59                     | 0.81              |
| 7:6:21:DA:N1       | 8:7:15:G:C2        | 2.49                     | 0.81              |
| 9:9:3:LEU:HD13     | 9:9:5:LEU:HG       | 1.62                     | 0.81              |
| 8:7:-18:G:H5''     | 17:D:1500:A:H62    | 1.40                     | 0.81              |
| 12:AB:65:PHE:CD2   | 12:AB:68:TYR:O     | 2.33                     | 0.81              |
| 14:AE:81:ARG:H     | 14:AE:81:ARG:HD2   | 1.45                     | 0.81              |
| 17:D:972:C:O2'     | 29:P:57:VAL:CG2    | 2.29                     | 0.81              |
| 21:H:267:TRP:CZ3   | 21:H:340:ARG:CG    | 2.63                     | 0.81              |
| 7:6:5:DT:P         | 14:AE:1172:LYS:HZ3 | 2.02                     | 0.81              |
| 12:AB:144:PHE:CE2  | 29:P:81:GLU:CG     | 2.62                     | 0.81              |
| 17:D:37:U:N3       | 17:D:397:A:N6      | 2.28                     | 0.81              |
| 10:B:54:U:H3       | 10:B:58:A:N6       | 1.77                     | 0.81              |
| 10:B:7:G:H4'       | 10:B:8:U:OP1       | 1.81                     | 0.81              |
| 10:B:76:A:H1'      | 40:a:2494:G:P      | 2.20                     | 0.81              |
| 10:A:22:G:H2'      | 10:A:23:C:C6       | 2.16                     | 0.80              |
| 17:D:1397:C:OP1    | 17:D:1397:C:H2'    | 1.81                     | 0.80              |
| 9:9:3:LEU:H        | 9:9:3:LEU:HD12     | 1.47                     | 0.80              |
| 9:9:50:VAL:HG22    | 38:Y:119:ALA:HB3   | 1.60                     | 0.80              |
| 10:B:22:G:H2'      | 10:B:23:C:C6       | 2.16                     | 0.80              |
| 10:B:58:A:O2'      | 10:B:59:A:H3'      | 1.82                     | 0.80              |
| 40:a:585:G:N7      | 65:z:6:ARG:NH1     | 2.29                     | 0.80              |
| 21:H:122:VAL:O     | 21:H:129:ALA:N     | 2.13                     | 0.80              |
| 23:J:162:ALA:CB    | 23:J:165:ARG:NH2   | 2.44                     | 0.80              |
| 38:Y:72:THR:OG1    | 38:Y:73:PRO:HD2    | 1.81                     | 0.80              |
| 12:AB:133:MET:SD   | 12:AB:146:GLY:N    | 2.54                     | 0.80              |
| 21:H:305:HIS:CD2   | 21:H:306:VAL:H     | 1.98                     | 0.80              |
| 23:J:162:ALA:CA    | 23:J:165:ARG:NH2   | 2.44                     | 0.80              |
| 10:B:56:C:C2'      | 10:B:57:A:H5''     | 2.11                     | 0.80              |
| 40:a:1019:U:H3     | 40:a:1142:A:N6     | 1.77                     | 0.80              |
| 53:n:125:ARG:O     | 53:n:127:ASN:ND2   | 2.14                     | 0.80              |
| 23:J:162:ALA:HA    | 23:J:165:ARG:NH2   | 1.95                     | 0.80              |
| 9:9:39:THR:HA      | 9:9:42:ARG:HD2     | 1.64                     | 0.80              |
| 12:AB:158:LEU:HD11 | 12:AB:175:PHE:CD1  | 2.17                     | 0.80              |
| 10:A:7:G:H4'       | 10:A:8:U:OP1       | 1.81                     | 0.80              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:Y:27:LEU:HD12   | 38:Y:27:LEU:O     | 1.81                     | 0.80              |
| 17:D:1329:A:P      | 37:X:28:THR:HB    | 2.22                     | 0.79              |
| 10:A:18:G:N2       | 10:A:58:A:C5      | 2.50                     | 0.79              |
| 21:H:270:ILE:CG2   | 21:H:337:GLU:HB3  | 2.12                     | 0.79              |
| 40:a:2297:A:N1     | 40:a:2321:U:O4    | 2.14                     | 0.79              |
| 40:a:2298:A:C4     | 40:a:2321:U:C5    | 2.70                     | 0.79              |
| 10:A:58:A:O2'      | 10:A:59:A:H3'     | 1.81                     | 0.79              |
| 46:g:18:CYS:HB3    | 46:g:40:CYS:CB    | 2.12                     | 0.79              |
| 9:9:78:GLY:N       | 9:9:79:PRO:HD2    | 1.97                     | 0.79              |
| 10:B:18:G:N2       | 10:B:58:A:C5      | 2.50                     | 0.79              |
| 40:a:2189:U:OP1    | 40:a:2189:U:O4'   | 2.00                     | 0.79              |
| 20:G:35:ARG:HD2    | 21:H:14:LYS:HD3   | 1.65                     | 0.78              |
| 20:G:16:PHE:CZ     | 21:H:41:GLY:O     | 2.36                     | 0.78              |
| 12:AB:169:THR:HG21 | 29:P:84:VAL:HG13  | 1.64                     | 0.78              |
| 40:a:2756:U:N3     | 40:a:2758:A:N6    | 2.32                     | 0.78              |
| 38:Y:32:VAL:HG13   | 38:Y:60:VAL:HG21  | 1.66                     | 0.78              |
| 12:AB:164:ILE:CG1  | 29:P:88:MET:CB    | 2.61                     | 0.78              |
| 10:B:5:G:H2'       | 10:B:6:G:H5'      | 1.66                     | 0.78              |
| 10:A:15:G:N1       | 10:A:20:U:O2      | 2.17                     | 0.78              |
| 21:H:123:GLU:HA    | 21:H:128:ARG:HA   | 1.63                     | 0.78              |
| 40:a:1021:A:H61    | 40:a:1141:U:H3    | 1.29                     | 0.78              |
| 46:g:16:CYS:HB2    | 46:g:37:CYS:HB3   | 1.63                     | 0.78              |
| 10:A:5:G:H2'       | 10:A:6:G:H5'      | 1.66                     | 0.78              |
| 49:j:4:LEU:HD23    | 49:j:29:VAL:HG11  | 1.65                     | 0.78              |
| 10:A:18:G:C5       | 10:A:57:A:C6      | 2.72                     | 0.77              |
| 12:AB:168:ALA:CB   | 29:P:88:MET:HA    | 2.10                     | 0.77              |
| 21:H:19:ARG:HD3    | 21:H:73:ASP:CG    | 2.09                     | 0.77              |
| 16:C:44:ILE:CD1    | 21:H:339:ARG:CG   | 2.62                     | 0.77              |
| 10:B:15:G:N1       | 10:B:20:U:O2      | 2.17                     | 0.77              |
| 10:B:18:G:C5       | 10:B:57:A:C6      | 2.72                     | 0.77              |
| 40:a:1406:U:O2'    | 40:a:1407:G:O5'   | 2.01                     | 0.77              |
| 9:9:50:VAL:CG2     | 38:Y:119:ALA:CB   | 2.59                     | 0.77              |
| 17:D:1358:U:C4     | 17:D:1363:A:N1    | 2.52                     | 0.77              |
| 40:a:1406:U:O2'    | 40:a:1407:G:P     | 2.41                     | 0.77              |
| 10:A:33:U:O3'      | 26:M:84:THR:OG1   | 2.02                     | 0.77              |
| 12:AB:133:MET:HG2  | 12:AB:146:GLY:C   | 2.03                     | 0.77              |
| 23:J:162:ALA:HB2   | 23:J:165:ARG:HH22 | 1.47                     | 0.77              |
| 7:6:18:DC:N3       | 8:7:17:G:N2       | 2.31                     | 0.77              |
| 12:AB:140:PRO:CG   | 29:P:79:PRO:CB    | 2.53                     | 0.77              |
| 38:Y:74:PRO:HG2    | 38:Y:77:VAL:HB    | 1.67                     | 0.77              |
| 40:a:2756:U:N3     | 40:a:2758:A:C6    | 2.53                     | 0.77              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:6:15:DC:C4       | 7:6:16:DC:N4      | 2.53                     | 0.77              |
| 9:9:31:ARG:NE      | 40:a:1054:A:C4'   | 2.48                     | 0.77              |
| 10:A:68:C:C3'      | 10:A:69:C:H5''    | 2.15                     | 0.77              |
| 12:AB:146:GLY:C    | 12:AB:163:SER:HG  | 1.90                     | 0.77              |
| 10:B:68:C:C3'      | 10:B:69:C:H5''    | 2.15                     | 0.77              |
| 10:A:76:A:H2'      | 40:a:2394:C:H42   | 1.47                     | 0.76              |
| 12:AB:146:GLY:HA2  | 12:AB:163:SER:CA  | 2.15                     | 0.76              |
| 12:AB:147:VAL:CG2  | 12:AB:163:SER:HG  | 1.99                     | 0.76              |
| 9:9:97:LYS:HD3     | 9:9:127:ALA:HA    | 1.68                     | 0.76              |
| 21:H:305:HIS:CD2   | 21:H:306:VAL:N    | 2.53                     | 0.76              |
| 9:9:11:ILE:HD11    | 9:9:62:ARG:HA     | 1.66                     | 0.76              |
| 21:H:109:THR:HA    | 21:H:153:GLU:HA   | 1.68                     | 0.76              |
| 40:a:2013:A:H61    | 40:a:2613:U:H3    | 1.31                     | 0.75              |
| 4:3:36:VAL:HG11    | 4:3:39:ILE:HD12   | 1.68                     | 0.75              |
| 9:9:31:ARG:CD      | 40:a:1054:A:C5'   | 2.58                     | 0.75              |
| 17:D:197:A:N6      | 17:D:221:C:H4'    | 2.01                     | 0.75              |
| 40:a:2298:A:C4     | 40:a:2321:U:H5    | 2.05                     | 0.75              |
| 46:g:18:CYS:CB     | 46:g:40:CYS:HB3   | 2.16                     | 0.75              |
| 9:9:27:VAL:HG23    | 9:9:83:ALA:HB3    | 1.67                     | 0.75              |
| 9:9:60:LEU:HD23    | 9:9:64:VAL:HG21   | 1.67                     | 0.75              |
| 12:AB:146:GLY:CA   | 12:AB:163:SER:CB  | 2.64                     | 0.75              |
| 63:x:31:THR:O      | 63:x:102:ARG:NH1  | 2.19                     | 0.75              |
| 24:K:137:VAL:O     | 24:K:140:THR:OG1  | 2.04                     | 0.75              |
| 29:P:24:GLU:OE2    | 29:P:90:LEU:HD11  | 1.87                     | 0.75              |
| 14:AE:59:ALA:HB1   | 14:AE:71:LEU:CD2  | 2.15                     | 0.75              |
| 12:AB:158:LEU:HD11 | 12:AB:175:PHE:CE1 | 2.21                     | 0.75              |
| 10:A:70:G:H2'      | 10:A:71:C:C5'     | 2.11                     | 0.74              |
| 9:9:78:GLY:N       | 9:9:79:PRO:CD     | 2.51                     | 0.74              |
| 20:G:35:ARG:HG3    | 21:H:10:GLU:OE2   | 1.86                     | 0.74              |
| 21:H:109:THR:CA    | 21:H:153:GLU:HA   | 2.18                     | 0.74              |
| 38:Y:85:ILE:H      | 38:Y:85:ILE:HD12  | 1.52                     | 0.74              |
| 21:H:162:LYS:CA    | 21:H:298:GLU:OE2  | 2.17                     | 0.74              |
| 10:A:32:C:C1'      | 26:M:144:MET:HE1  | 2.16                     | 0.74              |
| 16:C:44:ILE:HD13   | 21:H:339:ARG:HG3  | 1.70                     | 0.74              |
| 10:A:70:G:C3'      | 10:A:71:C:H5''    | 2.18                     | 0.74              |
| 12:AB:53:ARG:HB3   | 12:AB:123:ARG:HD3 | 1.68                     | 0.74              |
| 12:AB:150:GLU:HB3  | 12:AB:159:LYS:HB3 | 1.69                     | 0.74              |
| 10:B:18:G:H1'      | 10:B:58:A:C2      | 2.23                     | 0.74              |
| 9:9:52:MET:HG3     | 9:9:95:LEU:HD11   | 1.68                     | 0.74              |
| 12:AB:144:PHE:CE1  | 29:P:85:ASP:HB3   | 2.23                     | 0.74              |
| 20:G:19:GLN:CG     | 21:H:76:GLU:HB2   | 2.18                     | 0.74              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:a:1021:A:N1     | 40:a:1141:U:C4    | 2.55                     | 0.74              |
| 21:H:131:LEU:CB    | 21:H:166:VAL:C    | 2.60                     | 0.74              |
| 10:A:41:C:H1'      | 26:M:143:ARG:HH12 | 1.52                     | 0.73              |
| 21:H:110:GLY:CA    | 21:H:153:GLU:O    | 2.36                     | 0.73              |
| 10:A:6:G:O2'       | 10:A:7:G:O5'      | 2.05                     | 0.73              |
| 10:A:18:G:O2'      | 10:A:60:U:C2      | 2.41                     | 0.73              |
| 12:AB:144:PHE:CZ   | 29:P:85:ASP:OD2   | 2.40                     | 0.73              |
| 21:H:304:VAL:HG12  | 21:H:309:MET:SD   | 2.28                     | 0.73              |
| 12:AB:165:PHE:CE2  | 29:P:89:ARG:HG3   | 2.23                     | 0.73              |
| 12:AB:158:LEU:HD21 | 12:AB:175:PHE:CZ  | 2.24                     | 0.73              |
| 14:AE:47:ARG:CZ    | 29:P:81:GLU:OE1   | 2.36                     | 0.73              |
| 10:A:41:C:O4'      | 26:M:143:ARG:NH1  | 2.20                     | 0.73              |
| 10:B:70:G:C3'      | 10:B:71:C:H5''    | 2.17                     | 0.73              |
| 10:A:33:U:H5''     | 26:M:84:THR:CG2   | 2.19                     | 0.73              |
| 10:B:18:G:O2'      | 10:B:60:U:C2      | 2.41                     | 0.73              |
| 17:D:1228:C:OP1    | 37:X:107:ARG:NH1  | 2.21                     | 0.73              |
| 10:A:18:G:H1'      | 10:A:58:A:C2      | 2.23                     | 0.73              |
| 14:AE:77:ARG:NE    | 14:AE:77:ARG:HA   | 2.04                     | 0.73              |
| 38:Y:36:GLU:OE1    | 38:Y:36:GLU:HA    | 1.88                     | 0.73              |
| 17:D:517:G:O2'     | 17:D:530:G:H4'    | 1.88                     | 0.73              |
| 10:B:6:G:O2'       | 10:B:7:G:O5'      | 2.05                     | 0.73              |
| 14:AE:81:ARG:HD2   | 14:AE:81:ARG:N    | 2.03                     | 0.73              |
| 31:R:86:ARG:HG3    | 31:R:86:ARG:O     | 1.89                     | 0.72              |
| 12:AB:54:GLY:HA3   | 12:AB:59:LYS:HE3  | 1.70                     | 0.72              |
| 10:B:76:A:H1'      | 40:a:2494:G:OP1   | 1.88                     | 0.72              |
| 17:D:827:U:H3      | 17:D:872:A:N6     | 1.87                     | 0.72              |
| 40:a:1839:G:H1'    | 40:a:1927:A:N9    | 2.03                     | 0.72              |
| 40:a:1839:G:C1'    | 40:a:1927:A:C1'   | 2.67                     | 0.72              |
| 20:G:19:GLN:CD     | 21:H:76:GLU:HB2   | 2.08                     | 0.72              |
| 8:7:-12:U:N3       | 17:D:1196:A:C8    | 2.57                     | 0.72              |
| 10:B:76:A:H2'      | 10:B:76:A:N3      | 2.03                     | 0.72              |
| 28:O:84:THR:HG21   | 28:O:103:PHE:HB3  | 1.71                     | 0.72              |
| 12:AB:113:ASN:O    | 12:AB:117:GLN:HG3 | 1.89                     | 0.72              |
| 7:6:21:DA:C6       | 8:7:15:G:N2       | 2.57                     | 0.72              |
| 8:7:-3:U:H5''      | 8:7:-3:U:C6       | 2.24                     | 0.72              |
| 16:C:12:ARG:HB2    | 21:H:264:GLU:CB   | 2.20                     | 0.72              |
| 21:H:19:ARG:HB2    | 21:H:73:ASP:OD2   | 1.88                     | 0.72              |
| 12:AB:164:ILE:HG22 | 29:P:88:MET:SD    | 2.29                     | 0.72              |
| 20:G:19:GLN:OE1    | 21:H:75:VAL:O     | 1.85                     | 0.72              |
| 10:B:72:A:C3'      | 10:B:73:A:H5''    | 2.20                     | 0.72              |
| 20:G:16:PHE:CB     | 21:H:43:LYS:HA    | 2.20                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:A:72:A:C3'      | 10:A:73:A:H5''     | 2.20                     | 0.72              |
| 12:AB:148:VAL:HG13 | 12:AB:148:VAL:O    | 1.89                     | 0.72              |
| 21:H:267:TRP:CE3   | 21:H:340:ARG:CG    | 2.72                     | 0.72              |
| 40:a:67:U:C4       | 40:a:74:A:N6       | 2.57                     | 0.72              |
| 46:g:18:CYS:CB     | 46:g:40:CYS:CB     | 2.69                     | 0.71              |
| 14:AE:64:PRO:HG3   | 14:AE:90:VAL:CG1   | 2.20                     | 0.71              |
| 10:A:46:G:H1'      | 10:A:47:U:C5       | 2.25                     | 0.71              |
| 10:B:70:G:H2'      | 10:B:71:C:C5'      | 2.11                     | 0.71              |
| 17:D:1308:U:C3'    | 37:X:98:ARG:HH21   | 1.92                     | 0.71              |
| 17:D:1308:U:O5'    | 37:X:98:ARG:HG3    | 1.90                     | 0.71              |
| 40:a:2314:A:C1'    | 53:n:155:THR:HG21  | 2.21                     | 0.71              |
| 12:AB:145:ASN:O    | 12:AB:162:VAL:CG1  | 2.37                     | 0.71              |
| 8:7:14:U:H4'       | 14:AE:322:ARG:CZ   | 2.21                     | 0.71              |
| 10:B:46:G:H1'      | 10:B:47:U:C5       | 2.25                     | 0.71              |
| 40:a:1913:A:OP2    | 40:a:1913:A:H3'    | 1.89                     | 0.71              |
| 10:B:18:G:C5       | 10:B:57:A:N6       | 2.59                     | 0.71              |
| 9:9:77:VAL:HG12    | 9:9:82:ILE:HG21    | 1.71                     | 0.71              |
| 12:AB:144:PHE:CZ   | 29:P:81:GLU:HG2    | 2.26                     | 0.71              |
| 21:H:267:TRP:CE3   | 21:H:340:ARG:HG2   | 2.25                     | 0.71              |
| 6:5:100:DA:H5'     | 14:AE:278:ARG:HH11 | 1.56                     | 0.70              |
| 14:AE:68:TYR:HA    | 14:AE:92:VAL:HG23  | 1.72                     | 0.70              |
| 14:AE:59:ALA:HB1   | 14:AE:71:LEU:HD22  | 1.71                     | 0.70              |
| 21:H:70:VAL:HA     | 21:H:85:SER:CB     | 2.20                     | 0.70              |
| 21:H:86:ARG:O      | 21:H:89:ALA:HB3    | 1.91                     | 0.70              |
| 10:B:76:A:H2'      | 40:a:2493:U:H5''   | 1.72                     | 0.70              |
| 9:9:18:VAL:HA      | 9:9:86:MET:HE2     | 1.71                     | 0.70              |
| 10:A:41:C:C1'      | 26:M:143:ARG:NH1   | 2.55                     | 0.70              |
| 40:a:742:A:H2'     | 40:a:743:A:C8      | 2.26                     | 0.70              |
| 37:X:96:PRO:HG2    | 37:X:102:THR:CG2   | 2.21                     | 0.70              |
| 10:A:18:G:C5       | 10:A:57:A:N6       | 2.59                     | 0.70              |
| 10:A:32:C:C1'      | 26:M:144:MET:CE    | 2.69                     | 0.70              |
| 21:H:19:ARG:HD3    | 21:H:73:ASP:OD1    | 1.92                     | 0.70              |
| 47:h:146:MET:HE3   | 47:h:154:LEU:HD21  | 1.74                     | 0.70              |
| 9:9:58:THR:HG21    | 9:9:81:LEU:HG      | 1.74                     | 0.70              |
| 40:a:2310:C:O2'    | 53:n:74:VAL:CG1    | 2.40                     | 0.70              |
| 8:7:-12:U:O4       | 17:D:1196:A:N9     | 2.24                     | 0.70              |
| 12:AB:141:PHE:CE1  | 29:P:84:VAL:HG21   | 2.27                     | 0.70              |
| 17:D:972:C:O2'     | 29:P:57:VAL:HG23   | 1.92                     | 0.70              |
| 11:AA:909:LYS:HE3  | 29:P:31:ARG:NH1    | 2.07                     | 0.69              |
| 12:AB:164:ILE:HG13 | 29:P:88:MET:HB2    | 1.74                     | 0.69              |
| 8:7:2:U:OP1        | 14:AE:77:ARG:NH1   | 2.25                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:A:11:A:H2'      | 10:A:12:G:O4'      | 1.92                     | 0.69              |
| 10:A:15:G:H2'      | 10:A:15:G:N3       | 2.06                     | 0.69              |
| 9:9:3:LEU:HD12     | 9:9:3:LEU:N        | 2.05                     | 0.69              |
| 12:AB:127:LEU:HD12 | 12:AB:153:TYR:OH   | 1.90                     | 0.69              |
| 12:AB:171:VAL:HG21 | 29:P:102:LEU:CB    | 2.09                     | 0.69              |
| 17:D:915:A:N6      | 17:D:916:U:C4      | 2.60                     | 0.69              |
| 17:D:1309:G:H8     | 37:X:98:ARG:NH2    | 1.89                     | 0.69              |
| 21:H:70:VAL:HA     | 21:H:85:SER:CA     | 2.22                     | 0.69              |
| 12:AB:164:ILE:CG1  | 29:P:88:MET:HB2    | 2.22                     | 0.69              |
| 10:B:11:A:H2'      | 10:B:12:G:O4'      | 1.92                     | 0.69              |
| 21:H:19:ARG:HD3    | 21:H:73:ASP:OD2    | 1.92                     | 0.69              |
| 8:7:12:G:H1'       | 14:AE:253:VAL:CG1  | 2.20                     | 0.69              |
| 8:7:14:U:H4'       | 14:AE:322:ARG:NE   | 2.08                     | 0.69              |
| 9:9:31:ARG:HD2     | 40:a:1054:A:C5'    | 2.22                     | 0.69              |
| 10:A:16:C:O2       | 40:a:2181:U:C5'    | 2.40                     | 0.69              |
| 40:a:1839:G:C4     | 40:a:1927:A:C4     | 2.81                     | 0.69              |
| 38:Y:21:PRO:CB     | 38:Y:22:PRO:HD3    | 2.22                     | 0.69              |
| 17:D:563:A:N1      | 17:D:884:U:C4      | 2.60                     | 0.69              |
| 40:a:927:A:H2'     | 40:a:928:A:C8      | 2.28                     | 0.69              |
| 40:a:1021:A:H3'    | 40:a:1021:A:N3     | 2.07                     | 0.69              |
| 9:9:50:VAL:HG13    | 38:Y:119:ALA:CB    | 2.22                     | 0.69              |
| 11:AA:65:ASN:HB3   | 11:AA:105:TYR:HB2  | 1.73                     | 0.69              |
| 10:B:15:G:H2'      | 10:B:15:G:N3       | 2.06                     | 0.69              |
| 40:a:1596:A:H2'    | 40:a:1597:A:C8     | 2.28                     | 0.69              |
| 8:7:14:U:H4'       | 14:AE:322:ARG:NH1  | 2.08                     | 0.69              |
| 17:D:13:U:O4       | 17:D:21:G:C2       | 2.46                     | 0.69              |
| 9:9:73:LYS:HB2     | 9:9:117:LEU:HD21   | 1.75                     | 0.68              |
| 40:a:2756:U:C4     | 40:a:2758:A:N6     | 2.61                     | 0.68              |
| 7:6:5:DT:P         | 14:AE:1172:LYS:HZ1 | 2.13                     | 0.68              |
| 7:6:21:DA:C2       | 8:7:15:G:N2        | 2.61                     | 0.68              |
| 14:AE:1033:GLY:HA3 | 14:AE:1081:VAL:O   | 1.93                     | 0.68              |
| 37:X:96:PRO:CG     | 37:X:102:THR:CG2   | 2.71                     | 0.68              |
| 17:D:1227:A:H5'    | 37:X:110:LYS:HZ2   | 1.58                     | 0.68              |
| 17:D:37:U:H3       | 17:D:397:A:N6      | 1.90                     | 0.68              |
| 21:H:267:TRP:CD2   | 21:H:340:ARG:CG    | 2.76                     | 0.68              |
| 1:0:80:ARG:NH2     | 40:a:572:A:OP2     | 2.25                     | 0.68              |
| 40:a:2310:C:O2'    | 53:n:74:VAL:HG12   | 1.94                     | 0.68              |
| 9:9:11:ILE:CD1     | 9:9:62:ARG:HD3     | 2.24                     | 0.68              |
| 38:Y:58:ILE:HD13   | 38:Y:58:ILE:N      | 2.09                     | 0.68              |
| 38:Y:116:MET:HB3   | 38:Y:124:MET:HG2   | 1.76                     | 0.68              |
| 21:H:117:LYS:CB    | 21:H:279:LYS:O     | 2.41                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:AB:144:PHE:HE2 | 29:P:81:GLU:CG     | 2.05                     | 0.67              |
| 37:X:96:PRO:CG    | 37:X:102:THR:HG22  | 2.25                     | 0.67              |
| 10:A:5:G:H2'      | 10:A:6:G:C5'       | 2.24                     | 0.67              |
| 21:H:110:GLY:HA3  | 21:H:153:GLU:O     | 1.93                     | 0.67              |
| 6:5:100:DA:H5'    | 14:AE:278:ARG:HH12 | 1.54                     | 0.67              |
| 12:AB:133:MET:SD  | 12:AB:163:SER:CB   | 2.81                     | 0.67              |
| 12:AB:133:MET:HE2 | 12:AB:163:SER:HB3  | 1.76                     | 0.67              |
| 8:7:-12:U:O4      | 17:D:1196:A:O4'    | 2.13                     | 0.67              |
| 14:AE:59:ALA:HB2  | 14:AE:71:LEU:HD21  | 1.74                     | 0.67              |
| 7:6:8:DC:C6       | 7:6:9:DT:H72       | 2.29                     | 0.67              |
| 8:7:-10:U:O2'     | 24:K:33:PHE:HE1    | 1.76                     | 0.67              |
| 9:9:43:LYS:HD2    | 9:9:43:LYS:O       | 1.94                     | 0.67              |
| 40:a:1779:U:H5    | 40:a:1784:A:N7     | 1.93                     | 0.67              |
| 9:9:118:ILE:HB    | 9:9:119:PRO:HD3    | 1.76                     | 0.67              |
| 20:G:19:GLN:CG    | 21:H:75:VAL:CG2    | 2.70                     | 0.67              |
| 10:A:19:G:N2      | 40:a:2112:G:C8     | 2.62                     | 0.67              |
| 40:a:1153:C:OP1   | 65:z:92:ARG:NH1    | 2.27                     | 0.67              |
| 12:AB:146:GLY:CA  | 12:AB:163:SER:OG   | 2.43                     | 0.67              |
| 10:B:21:A:H4'     | 10:B:21:A:OP1      | 1.95                     | 0.67              |
| 21:H:270:ILE:HG23 | 21:H:337:GLU:HB3   | 1.77                     | 0.67              |
| 12:AB:142:ALA:O   | 12:AB:143:ASP:HB2  | 1.94                     | 0.66              |
| 10:B:5:G:H2'      | 10:B:6:G:C5'       | 2.24                     | 0.66              |
| 40:a:1920:C:O5'   | 40:a:1920:C:H6     | 1.77                     | 0.66              |
| 9:9:67:THR:N      | 9:9:68:PRO:CD      | 2.58                     | 0.66              |
| 13:AD:48:LEU:HB2  | 13:AD:183:ILE:HD11 | 1.76                     | 0.66              |
| 22:I:75:ILE:O     | 22:I:75:ILE:HD13   | 1.95                     | 0.66              |
| 38:Y:14:ALA:HB2   | 38:Y:54:ILE:HD12   | 1.76                     | 0.66              |
| 21:H:70:VAL:HA    | 21:H:85:SER:HA     | 1.77                     | 0.66              |
| 12:AB:134:VAL:CG2 | 12:AB:160:VAL:HG11 | 2.25                     | 0.66              |
| 9:9:50:VAL:CG1    | 38:Y:119:ALA:HB3   | 2.26                     | 0.66              |
| 10:A:66:C:H6      | 10:A:66:C:H5'      | 1.60                     | 0.66              |
| 21:H:162:LYS:CB   | 21:H:298:GLU:OE1   | 2.44                     | 0.66              |
| 12:AB:144:PHE:CE2 | 29:P:81:GLU:HG2    | 2.30                     | 0.66              |
| 40:a:1839:G:H8    | 40:a:1927:A:H1'    | 1.54                     | 0.66              |
| 10:A:56:C:C5      | 40:a:2168:G:C6     | 2.83                     | 0.66              |
| 12:AB:128:PHE:HE1 | 12:AB:180:LYS:HB2  | 1.59                     | 0.66              |
| 9:9:60:LEU:HA     | 9:9:64:VAL:HB      | 1.77                     | 0.66              |
| 9:9:61:ARG:NH1    | 40:a:1047:G:N7     | 2.44                     | 0.66              |
| 12:AB:48:GLU:HB3  | 12:AB:62:ARG:HG2   | 1.76                     | 0.66              |
| 10:B:37:A:H3'     | 10:B:37:A:OP2      | 1.96                     | 0.66              |
| 17:D:1308:U:H5''  | 37:X:98:ARG:HG2    | 1.78                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:H:110:GLY:N    | 21:H:153:GLU:C     | 2.53                     | 0.66              |
| 8:7:14:U:C4'      | 14:AE:322:ARG:NH1  | 2.59                     | 0.65              |
| 12:AB:144:PHE:CE1 | 29:P:85:ASP:CB     | 2.79                     | 0.65              |
| 10:B:76:A:H1'     | 40:a:2493:U:O3'    | 1.97                     | 0.65              |
| 55:p:24:ILE:HD13  | 55:p:72:LEU:HD21   | 1.77                     | 0.65              |
| 9:9:11:ILE:HG13   | 9:9:65:GLU:HB3     | 1.79                     | 0.65              |
| 10:B:66:C:H5'     | 10:B:66:C:H6       | 1.60                     | 0.65              |
| 11:AA:896:THR:HB  | 11:AA:897:PRO:HD2  | 1.79                     | 0.65              |
| 14:AE:79:LYS:CA   | 14:AE:81:ARG:HH12  | 1.96                     | 0.65              |
| 21:H:85:SER:O     | 21:H:88:LYS:CB     | 2.45                     | 0.65              |
| 40:a:1839:G:C8    | 40:a:1927:A:C1'    | 2.74                     | 0.65              |
| 12:AB:44:VAL:CG1  | 12:AB:45:PRO:CD    | 2.74                     | 0.65              |
| 10:B:22:G:H2'     | 10:B:23:C:H6       | 1.62                     | 0.65              |
| 17:D:1227:A:H5'   | 37:X:110:LYS:HZ1   | 1.61                     | 0.65              |
| 21:H:52:GLN:O     | 21:H:53:PHE:CD1    | 2.50                     | 0.65              |
| 10:A:32:C:C4'     | 26:M:144:MET:CE    | 2.66                     | 0.65              |
| 14:AE:84:ILE:HG22 | 14:AE:91:GLU:HG3   | 1.79                     | 0.65              |
| 17:D:197:A:C6     | 17:D:221:C:C4'     | 2.80                     | 0.65              |
| 54:o:26:HIS:CE1   | 54:o:48:ALA:HB2    | 2.32                     | 0.65              |
| 10:A:21:A:H4'     | 10:A:21:A:OP1      | 1.95                     | 0.65              |
| 21:H:110:GLY:H    | 21:H:153:GLU:CA    | 2.08                     | 0.65              |
| 37:X:96:PRO:HG3   | 37:X:102:THR:HG22  | 1.78                     | 0.65              |
| 40:a:1082:U:N3    | 40:a:1086:A:N6     | 2.45                     | 0.65              |
| 9:9:29:ASP:HB2    | 9:9:56:ARG:HD3     | 1.79                     | 0.65              |
| 10:B:56:C:H5'     | 53:n:80:ARG:NH2    | 2.10                     | 0.65              |
| 20:G:16:PHE:HZ    | 21:H:41:GLY:O      | 1.77                     | 0.65              |
| 10:A:22:G:H2'     | 10:A:23:C:H6       | 1.62                     | 0.65              |
| 12:AB:148:VAL:CA  | 12:AB:160:VAL:HG22 | 2.26                     | 0.65              |
| 14:AE:85:CYS:SG   | 67:AE:1502:ZN:ZN   | 1.79                     | 0.65              |
| 17:D:1308:U:O5'   | 37:X:98:ARG:CG     | 2.45                     | 0.65              |
| 21:H:332:VAL:HG12 | 21:H:334:ASP:H     | 1.62                     | 0.65              |
| 14:AE:79:LYS:C    | 14:AE:81:ARG:CZ    | 2.71                     | 0.64              |
| 21:H:118:GLY:C    | 21:H:133:GLY:CA    | 2.67                     | 0.64              |
| 38:Y:116:MET:HE2  | 38:Y:116:MET:HA    | 1.79                     | 0.64              |
| 40:a:1923:U:H2'   | 40:a:1923:U:OP2    | 1.96                     | 0.64              |
| 14:AE:58:CYS:SG   | 14:AE:59:ALA:N     | 2.69                     | 0.64              |
| 17:D:1227:A:OP2   | 37:X:110:LYS:NZ    | 2.29                     | 0.64              |
| 20:G:18:HIS:HA    | 21:H:43:LYS:CD     | 2.27                     | 0.64              |
| 32:S:47:LYS:O     | 32:S:50:THR:OG1    | 2.12                     | 0.64              |
| 8:7:-13:U:OP2     | 17:D:1397:C:N3     | 2.30                     | 0.64              |
| 8:7:-12:U:N3      | 17:D:1196:A:N7     | 2.44                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:A:41:C:C4'      | 26:M:143:ARG:NH1   | 2.60                     | 0.64              |
| 9:9:142:THR:HG21   | 39:Z:7:ILE:CD1     | 2.26                     | 0.64              |
| 17:D:1358:U:H3     | 17:D:1363:A:N6     | 1.96                     | 0.64              |
| 20:G:38:VAL:HG22   | 21:H:75:VAL:CG2    | 2.24                     | 0.64              |
| 58:s:114:LEU:HG    | 58:s:118:MET:HE3   | 1.78                     | 0.64              |
| 10:A:50:U:H2'      | 10:A:51:C:C6       | 2.33                     | 0.64              |
| 12:AB:133:MET:HE2  | 12:AB:163:SER:CB   | 2.27                     | 0.64              |
| 20:G:35:ARG:HH21   | 21:H:10:GLU:HG2    | 1.62                     | 0.64              |
| 35:V:25:ILE:HD11   | 35:V:61:ILE:HD11   | 1.77                     | 0.64              |
| 10:B:3:C:H2'       | 10:B:4:G:H8        | 1.62                     | 0.64              |
| 10:B:18:G:C8       | 10:B:57:A:C6       | 2.85                     | 0.64              |
| 20:G:19:GLN:CG     | 21:H:76:GLU:CB     | 2.76                     | 0.64              |
| 21:H:267:TRP:CE3   | 21:H:340:ARG:HG3   | 2.32                     | 0.64              |
| 40:a:1909:C:O5'    | 40:a:1909:C:H6     | 1.81                     | 0.64              |
| 11:AA:314:ASN:HD21 | 11:AA:348:SER:HA   | 1.62                     | 0.64              |
| 14:AE:79:LYS:C     | 14:AE:81:ARG:NH2   | 2.56                     | 0.64              |
| 10:B:75:C:OP1      | 40:a:2602:A:N9     | 2.30                     | 0.64              |
| 6:5:98:DA:C2'      | 6:5:99:DT:H72      | 2.28                     | 0.64              |
| 9:9:57:ASN:CG      | 9:9:62:ARG:CG      | 2.68                     | 0.64              |
| 17:D:1329:A:P      | 37:X:28:THR:CB     | 2.83                     | 0.64              |
| 21:H:267:TRP:CZ2   | 21:H:340:ARG:CG    | 2.68                     | 0.64              |
| 10:A:18:G:C8       | 10:A:57:A:C6       | 2.85                     | 0.64              |
| 12:AB:133:MET:CG   | 12:AB:146:GLY:CA   | 2.76                     | 0.64              |
| 12:AB:128:PHE:CE1  | 12:AB:180:LYS:HG3  | 2.33                     | 0.63              |
| 8:7:20:G:OP1       | 11:AA:1073:LYS:NZ  | 2.25                     | 0.63              |
| 10:B:50:U:H2'      | 10:B:51:C:C6       | 2.33                     | 0.63              |
| 21:H:135:LEU:CA    | 21:H:157:ILE:CB    | 2.74                     | 0.63              |
| 9:9:57:ASN:OD1     | 9:9:62:ARG:HD2     | 1.98                     | 0.63              |
| 10:A:56:C:O2       | 40:a:2112:G:C4     | 2.52                     | 0.63              |
| 12:AB:134:VAL:HG21 | 12:AB:160:VAL:HG21 | 1.80                     | 0.63              |
| 17:D:1358:U:N3     | 17:D:1363:A:N6     | 2.46                     | 0.63              |
| 55:p:121:ILE:HD12  | 55:p:141:ILE:HG22  | 1.79                     | 0.63              |
| 10:B:69:C:H2'      | 10:B:70:G:O4'      | 1.99                     | 0.63              |
| 23:J:162:ALA:CB    | 23:J:165:ARG:HH22  | 2.08                     | 0.63              |
| 40:a:1998:A:OP2    | 49:j:141:ARG:NH2   | 2.32                     | 0.63              |
| 6:5:100:DA:H4'     | 12:AB:16:SER:OG    | 1.98                     | 0.63              |
| 12:AB:128:PHE:CE1  | 12:AB:180:LYS:CG   | 2.82                     | 0.63              |
| 12:AB:148:VAL:HG21 | 12:AB:151:VAL:CG2  | 2.28                     | 0.63              |
| 17:D:1059:C:O2     | 29:P:55:PRO:HG3    | 1.99                     | 0.63              |
| 40:a:2303:G:N3     | 40:a:2314:A:C2     | 2.66                     | 0.63              |
| 10:A:69:C:H2'      | 10:A:70:G:O4'      | 1.99                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AA:1282:GLY:HA3 | 15:AF:17:PHE:HE1   | 1.63                     | 0.63              |
| 12:AB:140:PRO:O    | 29:P:81:GLU:HA     | 1.98                     | 0.63              |
| 10:A:3:C:H2'       | 10:A:4:G:H8        | 1.62                     | 0.63              |
| 21:H:267:TRP:CE2   | 21:H:340:ARG:CG    | 2.73                     | 0.63              |
| 8:7:12:G:O4'       | 14:AE:253:VAL:HG11 | 1.99                     | 0.63              |
| 1:0:40:MET:HE1     | 65:z:105:ALA:HB1   | 1.80                     | 0.63              |
| 8:7:-14:U:H5''     | 8:7:-14:U:H6       | 1.64                     | 0.63              |
| 21:H:49:PRO:CD     | 21:H:84:LEU:HD11   | 2.29                     | 0.63              |
| 21:H:304:VAL:HG12  | 21:H:304:VAL:O     | 1.99                     | 0.63              |
| 40:a:2189:U:O4'    | 40:a:2189:U:P      | 2.57                     | 0.63              |
| 10:A:31:G:O2'      | 26:M:144:MET:SD    | 2.56                     | 0.62              |
| 12:AB:140:PRO:HG3  | 29:P:79:PRO:CG     | 2.28                     | 0.62              |
| 12:AB:164:ILE:CG1  | 29:P:88:MET:HG3    | 2.29                     | 0.62              |
| 10:B:54:U:N3       | 10:B:58:A:N6       | 2.47                     | 0.62              |
| 21:H:270:ILE:CG2   | 21:H:337:GLU:CB    | 2.77                     | 0.62              |
| 26:M:23:LEU:O      | 26:M:27:VAL:HG13   | 1.99                     | 0.62              |
| 16:C:44:ILE:CD1    | 21:H:339:ARG:HG2   | 2.12                     | 0.62              |
| 17:D:827:U:N3      | 17:D:872:A:N6      | 2.45                     | 0.62              |
| 40:a:2013:A:N6     | 40:a:2613:U:N3     | 2.33                     | 0.62              |
| 40:a:2297:A:C2     | 40:a:2321:U:C4     | 2.86                     | 0.62              |
| 9:9:11:ILE:HD12    | 9:9:62:ARG:HD3     | 1.80                     | 0.62              |
| 9:9:78:GLY:H       | 9:9:79:PRO:CD      | 2.10                     | 0.62              |
| 17:D:1309:G:C8     | 37:X:98:ARG:NH2    | 2.66                     | 0.62              |
| 21:H:162:LYS:CB    | 21:H:298:GLU:OE2   | 2.45                     | 0.62              |
| 9:9:18:VAL:HG13    | 9:9:71:CYS:HB2     | 1.81                     | 0.62              |
| 12:AB:147:VAL:HG22 | 12:AB:163:SER:HG   | 1.63                     | 0.62              |
| 13:AD:211:ILE:HG12 | 13:AD:219:ARG:HH12 | 1.65                     | 0.62              |
| 8:7:2:U:OP1        | 14:AE:77:ARG:CZ    | 2.47                     | 0.62              |
| 12:AB:128:PHE:CZ   | 12:AB:180:LYS:HG3  | 2.33                     | 0.62              |
| 12:AB:164:ILE:CG1  | 29:P:88:MET:CG     | 2.77                     | 0.62              |
| 40:a:754:U:H2'     | 40:a:755:U:C6      | 2.35                     | 0.62              |
| 2:1:36:LEU:HD13    | 2:1:48:LYS:HA      | 1.80                     | 0.62              |
| 9:9:23:LEU:HB3     | 9:9:92:ALA:HA      | 1.81                     | 0.62              |
| 9:9:57:ASN:CG      | 9:9:62:ARG:HG2     | 2.25                     | 0.62              |
| 10:B:65:C:H2'      | 10:B:66:C:H5'      | 1.82                     | 0.62              |
| 40:a:1839:G:N9     | 40:a:1927:A:N9     | 2.48                     | 0.62              |
| 11:AA:845:LEU:HD21 | 11:AA:890:LYS:O    | 1.99                     | 0.62              |
| 16:C:29:LEU:O      | 16:C:33:ILE:HG23   | 2.00                     | 0.62              |
| 14:AE:47:ARG:CZ    | 29:P:81:GLU:CD     | 2.73                     | 0.61              |
| 10:B:42:G:H2'      | 10:B:43:A:H8       | 1.65                     | 0.61              |
| 17:D:37:U:O2       | 17:D:548:G:C2      | 2.52                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:G:19:GLN:HG3    | 21:H:75:VAL:CG2    | 2.23                     | 0.61              |
| 21:H:270:ILE:HG21  | 21:H:337:GLU:HB3   | 1.80                     | 0.61              |
| 40:a:1789:A:OP2    | 47:h:221:ARG:NH1   | 2.32                     | 0.61              |
| 12:AB:44:VAL:HG12  | 12:AB:45:PRO:CD    | 2.30                     | 0.61              |
| 12:AB:148:VAL:HA   | 12:AB:160:VAL:HG22 | 1.82                     | 0.61              |
| 21:H:280:LEU:N     | 21:H:330:VAL:O     | 2.32                     | 0.61              |
| 21:H:305:HIS:O     | 21:H:306:VAL:HB    | 2.00                     | 0.61              |
| 29:P:57:VAL:O      | 29:P:58:ASN:CG     | 2.43                     | 0.61              |
| 10:A:65:C:H2'      | 10:A:66:C:H5'      | 1.82                     | 0.61              |
| 10:B:56:C:C4'      | 53:n:80:ARG:NH2    | 2.64                     | 0.61              |
| 20:G:18:HIS:CA     | 21:H:43:LYS:HD2    | 2.29                     | 0.61              |
| 40:a:1021:A:C2     | 40:a:1141:U:O4     | 2.51                     | 0.61              |
| 7:6:15:DC:C4       | 7:6:16:DC:C4       | 2.89                     | 0.61              |
| 10:A:41:C:C1'      | 26:M:143:ARG:HH12  | 2.12                     | 0.61              |
| 16:C:44:ILE:CD1    | 21:H:339:ARG:HG3   | 2.28                     | 0.61              |
| 17:D:13:U:C5       | 17:D:20:U:O4       | 2.53                     | 0.61              |
| 21:H:110:GLY:N     | 21:H:153:GLU:O     | 2.32                     | 0.61              |
| 40:a:2720:U:OP1    | 64:y:53:ARG:NH2    | 2.34                     | 0.61              |
| 10:A:37:A:O2'      | 10:A:38:A:H5'      | 1.99                     | 0.61              |
| 11:AA:120:GLN:NE2  | 11:AA:490:GLN:OE1  | 2.32                     | 0.61              |
| 17:D:13:U:O4       | 17:D:20:U:C4       | 2.52                     | 0.61              |
| 34:U:21:VAL:HG21   | 34:U:60:TRP:CD1    | 2.36                     | 0.61              |
| 38:Y:32:VAL:HA     | 38:Y:60:VAL:HG11   | 1.81                     | 0.61              |
| 9:9:6:GLN:OE1      | 9:9:6:GLN:HA       | 2.00                     | 0.61              |
| 40:a:2885:G:N7     | 48:i:40:ARG:NH2    | 2.46                     | 0.61              |
| 14:AE:79:LYS:CA    | 14:AE:81:ARG:NH2   | 2.40                     | 0.61              |
| 20:G:19:GLN:HG3    | 21:H:76:GLU:HB2    | 1.82                     | 0.61              |
| 12:AB:148:VAL:HG21 | 12:AB:151:VAL:HG22 | 1.83                     | 0.61              |
| 10:B:3:C:H2'       | 10:B:4:G:C8        | 2.35                     | 0.61              |
| 17:D:1358:U:O4     | 17:D:1363:A:C2     | 2.47                     | 0.61              |
| 20:G:19:GLN:CD     | 21:H:75:VAL:HG22   | 2.25                     | 0.61              |
| 21:H:19:ARG:O      | 21:H:72:LEU:CB     | 2.41                     | 0.61              |
| 40:a:2297:A:C2     | 40:a:2321:U:C5     | 2.89                     | 0.61              |
| 3:2:50:LEU:HD23    | 44:e:26:PHE:CE1    | 2.35                     | 0.61              |
| 9:9:92:ALA:HB3     | 9:9:129:LEU:HB2    | 1.82                     | 0.61              |
| 11:AA:528:ARG:NH2  | 11:AA:576:SER:O    | 2.30                     | 0.61              |
| 14:AE:86:GLU:OE1   | 14:AE:86:GLU:N     | 2.34                     | 0.61              |
| 17:D:658:C:H1'     | 33:T:22:THR:HG21   | 1.83                     | 0.61              |
| 37:X:101:ARG:O     | 37:X:101:ARG:HD3   | 2.00                     | 0.61              |
| 40:a:1839:G:O4'    | 40:a:1927:A:H1'    | 1.97                     | 0.61              |
| 9:9:31:ARG:HH11    | 9:9:31:ARG:CG      | 2.14                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AA:887:VAL:HB   | 11:AA:913:VAL:HG23 | 1.82                     | 0.61              |
| 12:AB:164:ILE:CG1  | 29:P:88:MET:HA     | 2.14                     | 0.61              |
| 12:AB:168:ALA:HB2  | 29:P:88:MET:CA     | 2.20                     | 0.61              |
| 14:AE:888:CYS:SG   | 14:AE:889:ASP:N    | 2.74                     | 0.61              |
| 21:H:84:LEU:HD22   | 21:H:84:LEU:N      | 2.16                     | 0.61              |
| 10:A:41:C:H4'      | 26:M:143:ARG:CZ    | 2.31                     | 0.60              |
| 17:D:1218:C:H2'    | 17:D:1219:A:C8     | 2.36                     | 0.60              |
| 6:5:110:DA:N7      | 11:AA:183:TRP:CH2  | 2.69                     | 0.60              |
| 12:AB:144:PHE:HE2  | 29:P:81:GLU:HG3    | 1.59                     | 0.60              |
| 38:Y:54:ILE:O      | 38:Y:54:ILE:HG22   | 2.00                     | 0.60              |
| 40:a:84:A:N1       | 40:a:98:G:O2'      | 2.33                     | 0.60              |
| 10:A:34:C:P        | 26:M:84:THR:OG1    | 2.60                     | 0.60              |
| 12:AB:170:PRO:CG   | 29:P:100:ILE:O     | 2.48                     | 0.60              |
| 12:AB:171:VAL:HG21 | 29:P:102:LEU:HD23  | 1.82                     | 0.60              |
| 13:AC:45:ARG:HD3   | 13:AD:38:THR:HB    | 1.82                     | 0.60              |
| 9:9:47:GLU:HG3     | 9:9:95:LEU:HD21    | 1.83                     | 0.60              |
| 9:9:77:VAL:HG12    | 9:9:77:VAL:O       | 2.01                     | 0.60              |
| 11:AA:1072:ASN:ND2 | 11:AA:1111:GLN:OE1 | 2.34                     | 0.60              |
| 12:AB:133:MET:HG3  | 12:AB:163:SER:CB   | 2.31                     | 0.60              |
| 24:K:107:ALA:HB2   | 24:K:125:ALA:HB3   | 1.82                     | 0.60              |
| 38:Y:21:PRO:HB2    | 38:Y:22:PRO:CD     | 2.30                     | 0.60              |
| 39:Z:7:ILE:HG23    | 39:Z:7:ILE:O       | 2.01                     | 0.60              |
| 10:A:3:C:H2'       | 10:A:4:G:C8        | 2.36                     | 0.60              |
| 11:AA:55:SER:OG    | 11:AA:465:ARG:NH1  | 2.33                     | 0.60              |
| 17:D:1308:U:C5'    | 37:X:98:ARG:HG2    | 2.32                     | 0.60              |
| 21:H:117:LYS:CB    | 21:H:278:THR:HG23  | 2.32                     | 0.60              |
| 9:9:136:ILE:HD12   | 9:9:139:LEU:HD12   | 1.83                     | 0.60              |
| 10:A:54:U:N3       | 10:A:58:A:N6       | 2.48                     | 0.60              |
| 12:AB:151:VAL:HG12 | 12:AB:151:VAL:O    | 2.01                     | 0.60              |
| 12:AB:164:ILE:CG2  | 29:P:88:MET:HB2    | 2.31                     | 0.60              |
| 21:H:331:MET:N     | 21:H:331:MET:SD    | 2.75                     | 0.60              |
| 12:AB:169:THR:O    | 12:AB:169:THR:HG22 | 2.02                     | 0.60              |
| 14:AE:785:ASP:O    | 14:AE:789:LYS:HB2  | 2.01                     | 0.60              |
| 14:AE:814:CYS:SG   | 14:AE:883:ARG:NH2  | 2.74                     | 0.60              |
| 39:Z:20:VAL:O      | 39:Z:20:VAL:HG12   | 2.02                     | 0.60              |
| 14:AE:64:PRO:HG3   | 14:AE:90:VAL:HG12  | 1.83                     | 0.60              |
| 14:AE:1161:GLY:HA3 | 14:AE:1179:PRO:HA  | 1.83                     | 0.60              |
| 13:AD:112:ALA:HB3  | 13:AD:126:PRO:HA   | 1.83                     | 0.60              |
| 21:H:72:LEU:HD12   | 21:H:72:LEU:N      | 2.11                     | 0.60              |
| 21:H:305:HIS:CD2   | 21:H:307:SER:H     | 2.20                     | 0.60              |
| 14:AE:506:VAL:HG23 | 14:AE:628:GLY:HA3  | 1.83                     | 0.60              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:A:42:G:H2'       | 10:A:43:A:H8       | 1.65                     | 0.59              |
| 20:G:35:ARG:HD2     | 21:H:14:LYS:CD     | 2.32                     | 0.59              |
| 21:H:36:VAL:HB      | 21:H:48:ILE:HB     | 1.84                     | 0.59              |
| 10:A:33:U:H4'       | 26:M:84:THR:HB     | 1.82                     | 0.59              |
| 10:A:47:U:O2'       | 10:A:50:U:P        | 2.61                     | 0.59              |
| 10:A:35:A:H2'       | 10:A:36:U:C6       | 2.38                     | 0.59              |
| 11:AA:69:GLN:HE21   | 11:AA:101:ARG:HD2  | 1.67                     | 0.59              |
| 12:AB:45:PRO:HA     | 12:AB:65:PHE:HB2   | 1.85                     | 0.59              |
| 17:D:404:G:N7       | 23:J:2:ALA:HB3     | 2.17                     | 0.59              |
| 19:F:4:ILE:CD1      | 19:F:19:PHE:HA     | 2.33                     | 0.59              |
| 20:G:217:VAL:O      | 20:G:220:THR:HG22  | 2.02                     | 0.59              |
| 21:H:284:VAL:HG12   | 21:H:294:VAL:HB    | 1.84                     | 0.59              |
| 40:a:1921:G:O5'     | 40:a:1921:G:H8     | 1.84                     | 0.59              |
| 45:f:24:LEU:HD11    | 45:f:54:MET:HE2    | 1.83                     | 0.59              |
| 8:7:-11:U:H5''      | 8:7:-11:U:O2       | 2.03                     | 0.59              |
| 12:AB:164:ILE:HG21  | 29:P:88:MET:HB2    | 1.83                     | 0.59              |
| 14:AE:1275:LEU:HB3  | 14:AE:1278:GLU:HB2 | 1.83                     | 0.59              |
| 17:D:13:U:C2        | 17:D:915:A:N6      | 2.70                     | 0.59              |
| 26:M:69:VAL:HG23    | 26:M:100:ALA:HB1   | 1.83                     | 0.59              |
| 9:9:52:MET:HE3      | 9:9:52:MET:O       | 2.02                     | 0.59              |
| 10:A:34:C:P         | 26:M:84:THR:HG1    | 2.25                     | 0.59              |
| 11:AA:1142:ARG:NH1  | 11:AA:1161:LEU:O   | 2.36                     | 0.59              |
| 21:H:270:ILE:HG21   | 21:H:337:GLU:CB    | 2.32                     | 0.59              |
| 52:m:31:LEU:HD22    | 52:m:42:LEU:HD13   | 1.84                     | 0.59              |
| 8:7:14:U:C4'        | 14:AE:322:ARG:CZ   | 2.80                     | 0.59              |
| 14:AE:92:VAL:HG22   | 14:AE:92:VAL:O     | 2.01                     | 0.59              |
| 17:D:439:U:O2       | 17:D:440:C:C6      | 2.56                     | 0.59              |
| 8:7:-3:U:C6         | 8:7:-3:U:C5'       | 2.85                     | 0.59              |
| 9:9:78:GLY:H        | 9:9:79:PRO:HD2     | 1.68                     | 0.59              |
| 12:AB:144:PHE:CE1   | 29:P:85:ASP:CG     | 2.80                     | 0.59              |
| 14:AE:1221:LEU:HD22 | 14:AE:1306:LEU:HB2 | 1.85                     | 0.59              |
| 10:B:47:U:O2'       | 10:B:50:U:P        | 2.60                     | 0.59              |
| 10:A:58:A:H1'       | 10:A:60:U:C5       | 2.38                     | 0.59              |
| 17:D:321:A:N7       | 17:D:328:C:O2'     | 2.34                     | 0.59              |
| 40:a:70:G:H4'       | 40:a:71:A:OP1      | 2.02                     | 0.59              |
| 7:6:15:DC:N4        | 7:6:16:DC:H41      | 1.96                     | 0.58              |
| 9:9:19:ALA:HA       | 9:9:70:GLU:HG2     | 1.84                     | 0.58              |
| 9:9:61:ARG:CZ       | 40:a:1047:G:N7     | 2.67                     | 0.58              |
| 12:AB:19:GLU:OE2    | 12:AB:65:PHE:CD2   | 2.45                     | 0.58              |
| 12:AB:156:SER:O     | 12:AB:156:SER:OG   | 2.21                     | 0.58              |
| 12:AB:160:VAL:HG12  | 12:AB:162:VAL:H    | 1.67                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:D:563:A:N6      | 17:D:884:U:N3      | 2.51                     | 0.58              |
| 38:Y:112:LYS:HZ2   | 38:Y:112:LYS:HB3   | 1.68                     | 0.58              |
| 4:3:36:VAL:CG1     | 4:3:39:ILE:HD12    | 2.32                     | 0.58              |
| 9:9:54:VAL:O       | 9:9:54:VAL:HG22    | 2.03                     | 0.58              |
| 12:AB:133:MET:HG2  | 12:AB:146:GLY:H    | 1.68                     | 0.58              |
| 12:AB:148:VAL:CG2  | 12:AB:150:GLU:O    | 2.51                     | 0.58              |
| 18:E:25:ARG:HA     | 18:E:66:LEU:HD21   | 1.85                     | 0.58              |
| 10:A:76:A:H2'      | 40:a:2394:C:N4     | 2.11                     | 0.58              |
| 17:D:1225:A:H4'    | 36:W:78:ARG:NH1    | 2.18                     | 0.58              |
| 21:H:110:GLY:H     | 21:H:153:GLU:C     | 2.12                     | 0.58              |
| 37:X:104:THR:O     | 37:X:104:THR:HG22  | 2.03                     | 0.58              |
| 40:a:2000:C:OP1    | 62:w:5:LYS:NZ      | 2.36                     | 0.58              |
| 40:a:2314:A:O2'    | 53:n:155:THR:CG2   | 2.52                     | 0.58              |
| 11:AA:707:ALA:O    | 11:AA:711:ASP:HB2  | 2.04                     | 0.58              |
| 12:AB:141:PHE:HE1  | 12:AB:169:THR:HG21 | 1.68                     | 0.58              |
| 21:H:119:GLY:CA    | 21:H:131:LEU:O     | 2.46                     | 0.58              |
| 40:a:1590:A:H2'    | 40:a:1591:A:C8     | 2.38                     | 0.58              |
| 12:AB:146:GLY:HA3  | 12:AB:163:SER:N    | 2.02                     | 0.58              |
| 21:H:267:TRP:CH2   | 21:H:340:ARG:CB    | 2.86                     | 0.58              |
| 34:U:4:ILE:HG12    | 34:U:21:VAL:HG22   | 1.84                     | 0.58              |
| 49:j:33:ARG:NH1    | 49:j:53:GLY:O      | 2.36                     | 0.58              |
| 8:7:17:G:OP2       | 11:AA:540:ARG:NH1  | 2.37                     | 0.58              |
| 40:a:2572:A:C8     | 49:j:149:ASN:OD1   | 2.56                     | 0.58              |
| 7:6:18:DC:N4       | 8:7:17:G:H1        | 1.99                     | 0.58              |
| 11:AA:1254:VAL:O   | 14:AE:99:ARG:NH2   | 2.37                     | 0.58              |
| 12:AB:50:VAL:HG22  | 12:AB:62:ARG:HD2   | 1.86                     | 0.58              |
| 38:Y:7:TYR:HB2     | 38:Y:57:VAL:HG22   | 1.86                     | 0.58              |
| 6:5:99:DT:H2''     | 6:5:100:DA:H5''    | 1.85                     | 0.58              |
| 8:7:-12:U:O4       | 17:D:1196:A:C8     | 2.57                     | 0.58              |
| 10:A:76:A:C2'      | 40:a:2394:C:H42    | 2.16                     | 0.58              |
| 11:AA:838:CYS:HB2  | 11:AA:918:LEU:HD22 | 1.85                     | 0.58              |
| 21:H:118:GLY:C     | 21:H:133:GLY:HA2   | 2.27                     | 0.58              |
| 13:AC:82:LEU:HD11  | 13:AC:171:LEU:HD23 | 1.86                     | 0.58              |
| 17:D:1329:A:P      | 37:X:28:THR:OG1    | 2.62                     | 0.58              |
| 14:AE:1143:ASP:OD1 | 14:AE:1148:ARG:NH1 | 2.37                     | 0.58              |
| 10:B:60:U:P        | 10:B:61:C:H41      | 2.27                     | 0.58              |
| 21:H:119:GLY:HA3   | 21:H:132:PRO:C     | 2.28                     | 0.58              |
| 8:7:-14:U:H5''     | 8:7:-14:U:C6       | 2.39                     | 0.57              |
| 10:B:58:A:H1'      | 10:B:60:U:C5       | 2.38                     | 0.57              |
| 21:H:291:GLY:HA2   | 21:H:305:HIS:HA    | 1.86                     | 0.57              |
| 8:7:-12:U:O4       | 17:D:1196:A:C1'    | 2.52                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:7:-9:U:H3'       | 8:7:-9:U:H6        | 1.70                     | 0.57              |
| 12:AB:65:PHE:CZ    | 12:AB:70:LEU:CD1   | 2.86                     | 0.57              |
| 40:a:2245:U:O2'    | 40:a:2436:G:OP2    | 2.22                     | 0.57              |
| 10:A:18:G:C8       | 10:A:57:A:N6       | 2.69                     | 0.57              |
| 11:AA:13:LYS:HB2   | 11:AA:1180:MET:HE2 | 1.86                     | 0.57              |
| 12:AB:165:PHE:CE1  | 29:P:88:MET:HE3    | 2.38                     | 0.57              |
| 27:N:10:MET:HE3    | 27:N:61:LEU:HD11   | 1.87                     | 0.57              |
| 30:Q:67:ALA:HB2    | 30:Q:96:THR:HG23   | 1.86                     | 0.57              |
| 2:1:20:VAL:HG11    | 2:1:44:ALA:HA      | 1.86                     | 0.57              |
| 11:AA:1223:ARG:NH2 | 14:AE:721:SER:OG   | 2.38                     | 0.57              |
| 12:AB:167:ARG:NE   | 12:AB:167:ARG:HA   | 2.19                     | 0.57              |
| 20:G:148:LEU:HD22  | 20:G:151:ILE:HD11  | 1.86                     | 0.57              |
| 40:a:1839:G:N9     | 40:a:1927:A:C4     | 2.72                     | 0.57              |
| 12:AB:49:VAL:O     | 12:AB:49:VAL:HG13  | 2.04                     | 0.57              |
| 17:D:1526:G:OP2    | 19:F:42:THR:HG23   | 2.04                     | 0.57              |
| 46:g:16:CYS:HB3    | 46:g:37:CYS:HB3    | 1.86                     | 0.57              |
| 10:B:11:A:H2'      | 10:B:12:G:C8       | 2.40                     | 0.57              |
| 10:B:56:C:C5'      | 53:n:80:ARG:CZ     | 2.76                     | 0.57              |
| 20:G:19:GLN:NE2    | 21:H:75:VAL:HG22   | 2.19                     | 0.57              |
| 21:H:49:PRO:HD3    | 21:H:84:LEU:HD11   | 1.87                     | 0.57              |
| 21:H:330:VAL:HB    | 21:H:344:LEU:HD23  | 1.86                     | 0.57              |
| 24:K:56:VAL:O      | 24:K:60:ILE:HG23   | 2.04                     | 0.57              |
| 38:Y:78:LEU:HD13   | 38:Y:108:ILE:HG22  | 1.85                     | 0.57              |
| 60:u:77:ILE:HD11   | 60:u:108:ALA:HB1   | 1.87                     | 0.57              |
| 10:A:11:A:H2'      | 10:A:12:G:C8       | 2.40                     | 0.57              |
| 11:AA:1122:LYS:NZ  | 11:AA:1126:ASP:OD1 | 2.38                     | 0.57              |
| 12:AB:133:MET:SD   | 12:AB:146:GLY:CA   | 2.93                     | 0.57              |
| 11:AA:887:VAL:CB   | 11:AA:913:VAL:CG2  | 2.68                     | 0.57              |
| 12:AB:128:PHE:HE1  | 12:AB:180:LYS:CG   | 2.16                     | 0.57              |
| 12:AB:128:PHE:CE1  | 12:AB:180:LYS:HB2  | 2.38                     | 0.57              |
| 12:AB:144:PHE:CE2  | 29:P:81:GLU:O      | 2.58                     | 0.57              |
| 40:a:1818:U:OP2    | 47:h:156:ARG:NH1   | 2.38                     | 0.57              |
| 6:5:100:DA:C5'     | 14:AE:278:ARG:NH1  | 2.53                     | 0.57              |
| 12:AB:148:VAL:HG22 | 12:AB:150:GLU:O    | 2.03                     | 0.57              |
| 29:P:6:ILE:HG23    | 29:P:100:ILE:HG23  | 1.87                     | 0.57              |
| 12:AB:145:ASN:O    | 12:AB:162:VAL:C    | 2.48                     | 0.56              |
| 14:AE:741:ALA:O    | 14:AE:762:ASN:ND2  | 2.32                     | 0.56              |
| 17:D:496:A:N3      | 17:D:496:A:H2'     | 2.19                     | 0.56              |
| 38:Y:96:LYS:HE3    | 38:Y:136:GLY:HA3   | 1.87                     | 0.56              |
| 2:1:93:ALA:HB2     | 40:a:1614:A:C2     | 2.40                     | 0.56              |
| 9:9:34:THR:HG22    | 9:9:38:MET:HE3     | 1.85                     | 0.56              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:AA:845:LEU:CD2  | 11:AA:890:LYS:C     | 2.78                     | 0.56              |
| 10:B:6:G:HO2'      | 10:B:7:G:H8         | 1.54                     | 0.56              |
| 21:H:110:GLY:N     | 21:H:153:GLU:CA     | 2.67                     | 0.56              |
| 11:AA:839:VAL:HG12 | 11:AA:1049:ILE:HG12 | 1.87                     | 0.56              |
| 12:AB:47:GLU:HB3   | 12:AB:64:PHE:HD1    | 1.70                     | 0.56              |
| 10:B:32:C:OP2      | 28:O:130:ARG:NH2    | 2.38                     | 0.56              |
| 38:Y:137:LEU:N     | 38:Y:137:LEU:HD23   | 2.19                     | 0.56              |
| 40:a:580:U:O3'     | 65:z:31:VAL:HG13    | 2.05                     | 0.56              |
| 8:7:-20:A:H2'      | 8:7:-19:U:H6        | 1.70                     | 0.56              |
| 8:7:-9:U:H5''      | 24:K:56:VAL:HG21    | 1.87                     | 0.56              |
| 9:9:17:GLU:HB3     | 9:9:86:MET:HB2      | 1.87                     | 0.56              |
| 33:T:5:THR:O       | 33:T:8:THR:OG1      | 2.18                     | 0.56              |
| 38:Y:59:THR:HG22   | 38:Y:61:TYR:HE1     | 1.69                     | 0.56              |
| 8:7:-12:U:C4       | 17:D:1196:A:C8      | 2.93                     | 0.56              |
| 9:9:62:ARG:CG      | 9:9:62:ARG:HH21     | 2.14                     | 0.56              |
| 10:A:50:U:H2'      | 10:A:51:C:H6        | 1.69                     | 0.56              |
| 10:A:60:U:P        | 10:A:61:C:H41       | 2.27                     | 0.56              |
| 11:AA:516:ASP:OD1  | 11:AA:516:ASP:O     | 2.23                     | 0.56              |
| 46:g:16:CYS:CB     | 46:g:37:CYS:CB      | 2.82                     | 0.56              |
| 12:AB:133:MET:CG   | 12:AB:146:GLY:N     | 2.68                     | 0.56              |
| 7:6:21:DA:N6       | 8:7:15:G:H1         | 2.04                     | 0.56              |
| 9:9:35:VAL:HA      | 9:9:38:MET:HB2      | 1.88                     | 0.56              |
| 12:AB:128:PHE:HE1  | 12:AB:180:LYS:CB    | 2.18                     | 0.56              |
| 14:AE:144:TYR:OH   | 14:AE:293:ARG:NH2   | 2.37                     | 0.56              |
| 10:B:56:C:C5'      | 53:n:80:ARG:NH2     | 2.67                     | 0.56              |
| 21:H:71:ALA:O      | 21:H:72:LEU:CD1     | 2.42                     | 0.56              |
| 21:H:267:TRP:CH2   | 21:H:340:ARG:HB3    | 2.41                     | 0.56              |
| 42:c:31:PRO:HG2    | 42:c:33:LEU:HD13    | 1.87                     | 0.56              |
| 1:0:51:VAL:HG23    | 65:z:86:ALA:O       | 2.05                     | 0.56              |
| 10:A:56:C:C6       | 40:a:2168:G:C6      | 2.94                     | 0.56              |
| 21:H:305:HIS:HD2   | 21:H:306:VAL:H      | 1.49                     | 0.56              |
| 10:A:11:A:O5'      | 10:A:11:A:H8        | 1.89                     | 0.55              |
| 10:A:60:U:O2'      | 10:A:61:C:OP1       | 2.23                     | 0.55              |
| 38:Y:77:VAL:O      | 38:Y:77:VAL:HG12    | 2.05                     | 0.55              |
| 40:a:2249:U:H3'    | 40:a:2250:G:C5'     | 2.36                     | 0.55              |
| 11:AA:896:THR:HB   | 11:AA:897:PRO:CD    | 2.36                     | 0.55              |
| 13:AC:28:LEU:HD22  | 13:AC:201:LEU:HD23  | 1.88                     | 0.55              |
| 10:B:50:U:H2'      | 10:B:51:C:H6        | 1.69                     | 0.55              |
| 17:D:927:G:O2'     | 17:D:1503:A:N7      | 2.36                     | 0.55              |
| 38:Y:116:MET:HG3   | 38:Y:124:MET:HB3    | 1.89                     | 0.55              |
| 51:l:104:ALA:O     | 51:l:108:ILE:HG23   | 2.05                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:7:-18:G:H5''     | 17:D:1501:C:N4      | 2.21                     | 0.55              |
| 8:7:-13:U:H5'      | 17:D:1397:C:N3      | 2.22                     | 0.55              |
| 12:AB:147:VAL:CA   | 12:AB:163:SER:OG    | 2.54                     | 0.55              |
| 40:a:2314:A:O2'    | 53:n:155:THR:HG21   | 2.06                     | 0.55              |
| 10:A:6:G:HO2'      | 10:A:7:G:H8         | 1.55                     | 0.55              |
| 11:AA:818:VAL:HG22 | 11:AA:1096:ILE:HG12 | 1.87                     | 0.55              |
| 17:D:528:C:H6      | 17:D:528:C:H5''     | 1.71                     | 0.55              |
| 9:9:50:VAL:HG13    | 38:Y:119:ALA:HB3    | 1.88                     | 0.55              |
| 10:A:38:A:H2'      | 10:A:39:C:H5'       | 1.88                     | 0.55              |
| 39:Z:2:ILE:HB      | 39:Z:5:ASP:HB3      | 1.89                     | 0.55              |
| 51:l:130:LYS:HB2   | 51:l:133:LEU:HD12   | 1.89                     | 0.55              |
| 10:B:11:A:H8       | 10:B:11:A:O5'       | 1.89                     | 0.55              |
| 7:6:26:DT:H2''     | 7:6:27:DG:H5'       | 1.88                     | 0.55              |
| 8:7:14:U:C1'       | 14:AE:322:ARG:NH1   | 2.70                     | 0.55              |
| 21:H:45:GLU:OE1    | 21:H:45:GLU:N       | 2.40                     | 0.55              |
| 21:H:119:GLY:CA    | 21:H:133:GLY:CA     | 2.74                     | 0.55              |
| 11:AA:143:ARG:NH2  | 11:AA:512:SER:O     | 2.40                     | 0.55              |
| 21:H:154:PHE:CB    | 21:H:168:VAL:CB     | 2.85                     | 0.55              |
| 36:W:15:LEU:HD13   | 36:W:33:THR:HG21    | 1.88                     | 0.55              |
| 40:a:2683:C:OP1    | 64:y:51:ARG:NH2     | 2.32                     | 0.55              |
| 8:7:-3:U:O2        | 8:7:-3:U:H2'        | 2.06                     | 0.55              |
| 9:9:31:ARG:HG3     | 9:9:31:ARG:NH1      | 2.16                     | 0.55              |
| 11:AA:29:SER:O     | 11:AA:33:ASP:HB2    | 2.07                     | 0.55              |
| 24:K:99:ALA:HB1    | 24:K:103:THR:HG21   | 1.89                     | 0.55              |
| 61:v:66:ARG:NH1    | 61:v:104:GLU:OE1    | 2.39                     | 0.55              |
| 3:2:50:LEU:HD23    | 44:e:26:PHE:CZ      | 2.42                     | 0.54              |
| 8:7:-20:A:C4       | 8:7:-19:U:C5        | 2.95                     | 0.54              |
| 11:AA:1142:ARG:NH2 | 11:AA:1166:ASP:OD1  | 2.38                     | 0.54              |
| 12:AB:162:VAL:O    | 12:AB:162:VAL:HG12  | 2.07                     | 0.54              |
| 11:AA:985:GLU:HB3  | 11:AA:988:LYS:HB2   | 1.89                     | 0.54              |
| 12:AB:141:PHE:CE1  | 29:P:84:VAL:CG2     | 2.90                     | 0.54              |
| 17:D:439:U:O2      | 17:D:440:C:C5       | 2.61                     | 0.54              |
| 14:AE:1346:GLY:O   | 14:AE:1350:ASN:ND2  | 2.41                     | 0.54              |
| 8:7:-18:G:C4'      | 17:D:1500:A:H62     | 2.21                     | 0.54              |
| 9:9:51:TYR:CD1     | 9:9:51:TYR:C        | 2.85                     | 0.54              |
| 11:AA:360:LEU:HD13 | 11:AA:378:ARG:HH11  | 1.72                     | 0.54              |
| 11:AA:633:LEU:HD13 | 11:AA:644:LEU:HD23  | 1.89                     | 0.54              |
| 12:AB:133:MET:HG2  | 12:AB:146:GLY:N     | 2.21                     | 0.54              |
| 38:Y:19:PRO:HG2    | 38:Y:24:GLY:H       | 1.73                     | 0.54              |
| 63:x:35:ILE:HG21   | 63:x:71:ALA:HA      | 1.89                     | 0.54              |
| 7:6:2:DC:H2''      | 7:6:3:DC:C5         | 2.43                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:9:31:ARG:HD2     | 40:a:1054:A:C4'     | 2.29                     | 0.54              |
| 14:AE:968:ASN:HA   | 14:AE:1117:SER:HB2  | 1.90                     | 0.54              |
| 57:r:58:LEU:O      | 57:r:61:VAL:HG22    | 2.08                     | 0.54              |
| 8:7:-18:G:H3'      | 17:D:1500:A:N6      | 2.23                     | 0.54              |
| 14:AE:901:ARG:HH21 | 14:AE:906:GLY:HA2   | 1.73                     | 0.54              |
| 17:D:563:A:N6      | 17:D:884:U:H3       | 2.05                     | 0.54              |
| 17:D:961:U:O4      | 17:D:974:A:N1       | 2.40                     | 0.54              |
| 17:D:1515:G:H2'    | 17:D:1516:G:H8      | 1.72                     | 0.54              |
| 21:H:84:LEU:HD22   | 21:H:84:LEU:H       | 1.72                     | 0.54              |
| 21:H:290:TYR:C     | 21:H:305:HIS:O      | 2.47                     | 0.54              |
| 29:P:8:ILE:HD12    | 29:P:25:ILE:HD11    | 1.89                     | 0.54              |
| 40:a:2303:G:C4     | 40:a:2314:A:C2      | 2.95                     | 0.54              |
| 13:AC:100:LEU:HD23 | 13:AC:115:ILE:HG21  | 1.89                     | 0.54              |
| 14:AE:66:LYS:HB2   | 14:AE:69:GLU:CB     | 2.38                     | 0.54              |
| 21:H:116:VAL:C     | 21:H:279:LYS:HB2    | 2.33                     | 0.54              |
| 40:a:523:C:O2      | 40:a:554:U:O2'      | 2.25                     | 0.54              |
| 41:b:37:ILE:HD11   | 41:b:82:ILE:HD11    | 1.90                     | 0.54              |
| 8:7:-18:G:C3'      | 17:D:1500:A:N6      | 2.71                     | 0.54              |
| 9:9:58:THR:HG21    | 9:9:81:LEU:HA       | 1.90                     | 0.54              |
| 11:AA:684:ASN:OD1  | 11:AA:687:ARG:NH2   | 2.41                     | 0.54              |
| 10:B:17:C:O2       | 10:B:17:C:H2'       | 2.08                     | 0.54              |
| 7:6:22:DC:H4'      | 11:AA:508:SER:OG    | 2.07                     | 0.54              |
| 11:AA:903:ARG:HG3  | 11:AA:903:ARG:O     | 2.08                     | 0.54              |
| 14:AE:342:LEU:HD23 | 14:AE:1352:ILE:HG23 | 1.90                     | 0.54              |
| 14:AE:886:VAL:HG11 | 14:AE:1230:THR:HG21 | 1.89                     | 0.54              |
| 20:G:38:VAL:CG2    | 21:H:75:VAL:CG2     | 2.77                     | 0.54              |
| 21:H:52:GLN:OE1    | 21:H:86:ARG:CB      | 2.55                     | 0.54              |
| 38:Y:109:ALA:HB2   | 38:Y:128:ILE:HG13   | 1.89                     | 0.54              |
| 40:a:2192:U:H2'    | 40:a:2193:G:C8      | 2.43                     | 0.54              |
| 46:g:18:CYS:HB3    | 46:g:40:CYS:HB2     | 1.88                     | 0.54              |
| 12:AB:165:PHE:HE2  | 29:P:89:ARG:HG3     | 1.72                     | 0.54              |
| 13:AC:43:LEU:HD13  | 13:AC:217:ILE:HD11  | 1.90                     | 0.54              |
| 10:B:12:G:H2'      | 10:B:13:C:OP1       | 2.08                     | 0.54              |
| 17:D:769:G:H4'     | 17:D:1513:A:H4'     | 1.88                     | 0.54              |
| 40:a:1056:G:O2'    | 40:a:1103:A:N6      | 2.41                     | 0.54              |
| 10:A:56:C:C2       | 40:a:2112:G:C8      | 2.96                     | 0.53              |
| 14:AE:1000:GLY:HA3 | 14:AE:1026:PRO:HG2  | 1.90                     | 0.53              |
| 21:H:22:SER:N      | 21:H:69:ASP:OD2     | 2.40                     | 0.53              |
| 21:H:84:LEU:H      | 21:H:84:LEU:CD2     | 2.21                     | 0.53              |
| 31:R:80:ILE:HD12   | 31:R:97:THR:HG22    | 1.89                     | 0.53              |
| 63:x:27:VAL:HG21   | 63:x:40:ILE:HD12    | 1.89                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:A:12:G:H2'       | 10:A:13:C:OP1       | 2.08                     | 0.53              |
| 10:A:18:G:C2        | 10:A:58:A:C5        | 2.96                     | 0.53              |
| 11:AA:103:VAL:HB    | 11:AA:114:VAL:HG11  | 1.89                     | 0.53              |
| 12:AB:141:PHE:HE1   | 29:P:84:VAL:HG13    | 1.68                     | 0.53              |
| 13:AD:205:MET:HE3   | 13:AD:213:PRO:HB3   | 1.90                     | 0.53              |
| 17:D:13:U:C4        | 17:D:21:G:C2        | 2.96                     | 0.53              |
| 21:H:332:VAL:O      | 21:H:334:ASP:N      | 2.40                     | 0.53              |
| 51:l:108:ILE:HD11   | 51:l:180:LEU:HD13   | 1.89                     | 0.53              |
| 9:9:123:ILE:O       | 9:9:123:ILE:HG12    | 2.08                     | 0.53              |
| 10:A:16:C:O2        | 10:A:16:C:H2'       | 2.08                     | 0.53              |
| 11:AA:786:GLY:N     | 11:AA:789:THR:OG1   | 2.41                     | 0.53              |
| 17:D:13:U:C2        | 17:D:915:A:C6       | 2.95                     | 0.53              |
| 17:D:1329:A:OP1     | 37:X:28:THR:N       | 2.41                     | 0.53              |
| 21:H:321:VAL:HG13   | 21:H:322:VAL:HG23   | 1.90                     | 0.53              |
| 8:7:-10:U:O2        | 8:7:-10:U:H2'       | 2.06                     | 0.53              |
| 11:AA:628:HIS:HB3   | 11:AA:647:ARG:HH21  | 1.74                     | 0.53              |
| 14:AE:77:ARG:HD3    | 14:AE:78:LEU:H      | 1.73                     | 0.53              |
| 14:AE:514:THR:HG21  | 14:AE:596:LEU:HD12  | 1.90                     | 0.53              |
| 38:Y:12:VAL:HG12    | 38:Y:23:VAL:HG21    | 1.90                     | 0.53              |
| 51:l:131:THR:HG22   | 51:l:160:ALA:O      | 2.08                     | 0.53              |
| 4:3:13:VAL:CG2      | 4:3:39:ILE:HD13     | 2.39                     | 0.53              |
| 8:7:15:G:H2'        | 8:7:16:A:C8         | 2.43                     | 0.53              |
| 11:AA:1070:HIS:NE2  | 11:AA:1114:GLU:OE1  | 2.36                     | 0.53              |
| 10:B:18:G:C2        | 10:B:58:A:C5        | 2.97                     | 0.53              |
| 17:D:945:G:C2       | 17:D:946:A:C8       | 2.96                     | 0.53              |
| 17:D:1308:U:OP1     | 37:X:100:GLN:OE1    | 2.23                     | 0.53              |
| 21:H:24:VAL:HG12    | 21:H:69:ASP:H       | 1.74                     | 0.53              |
| 40:a:1406:U:HO2'    | 40:a:1407:G:C5'     | 2.11                     | 0.53              |
| 9:9:43:LYS:HG2      | 9:9:98:GLU:HG2      | 1.90                     | 0.53              |
| 9:9:139:LEU:HD11    | 39:Z:11:VAL:HG13    | 1.90                     | 0.53              |
| 11:AA:243:PRO:HB2   | 11:AA:274:ILE:HG23  | 1.90                     | 0.53              |
| 11:AA:1117:LEU:HD12 | 11:AA:1195:ILE:HG12 | 1.90                     | 0.53              |
| 12:AB:19:GLU:HG2    | 12:AB:44:VAL:CG1    | 2.39                     | 0.53              |
| 12:AB:157:ARG:NH2   | 12:AB:174:ASP:OD2   | 2.38                     | 0.53              |
| 14:AE:1175:LEU:O    | 14:AE:1187:GLU:HA   | 2.08                     | 0.53              |
| 17:D:673:A:H2'      | 17:D:674:G:C8       | 2.44                     | 0.53              |
| 17:D:1227:A:P       | 37:X:110:LYS:HZ2    | 2.31                     | 0.53              |
| 24:K:94:VAL:HG13    | 24:K:111:MET:HE1    | 1.91                     | 0.53              |
| 6:5:110:DA:N7       | 11:AA:183:TRP:HH2   | 2.06                     | 0.53              |
| 8:7:-8:U:H5''       | 8:7:-8:U:H6         | 1.73                     | 0.53              |
| 9:9:125:ARG:HA      | 9:9:125:ARG:CZ      | 2.38                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:AB:133:MET:CE    | 12:AB:163:SER:HB2   | 2.37                     | 0.53              |
| 13:AD:16:ILE:HG23   | 13:AD:26:VAL:HG22   | 1.91                     | 0.53              |
| 10:A:72:A:H2'       | 10:A:73:A:C5'       | 2.32                     | 0.53              |
| 40:a:811:U:H2'      | 60:u:21:ARG:HA      | 1.89                     | 0.53              |
| 40:a:1906:G:H5''    | 40:a:1906:G:H8      | 1.73                     | 0.53              |
| 2:1:59:GLU:CG       | 2:1:66:ILE:HD11     | 2.38                     | 0.53              |
| 14:AE:510:LEU:HD22  | 14:AE:601:ILE:HD12  | 1.91                     | 0.53              |
| 8:7:17:G:H2'        | 8:7:18:A:C8         | 2.44                     | 0.53              |
| 14:AE:1045:THR:O    | 14:AE:1067:ARG:NH2  | 2.41                     | 0.53              |
| 17:D:1228:C:OP2     | 37:X:110:LYS:NZ     | 2.41                     | 0.53              |
| 28:O:81:HIS:O       | 28:O:84:THR:OG1     | 2.23                     | 0.53              |
| 40:a:2328:A:H2'     | 40:a:2329:U:C6      | 2.44                     | 0.53              |
| 9:9:71:CYS:HA       | 9:9:117:LEU:HD13    | 1.91                     | 0.52              |
| 11:AA:855:PRO:HD2   | 11:AA:887:VAL:HG11  | 1.91                     | 0.52              |
| 12:AB:165:PHE:CD1   | 12:AB:165:PHE:N     | 2.74                     | 0.52              |
| 21:H:49:PRO:HD2     | 21:H:84:LEU:CD1     | 2.39                     | 0.52              |
| 21:H:135:LEU:CB     | 21:H:157:ILE:CB     | 2.87                     | 0.52              |
| 21:H:332:VAL:CG1    | 21:H:335:ILE:HG13   | 2.33                     | 0.52              |
| 38:Y:57:VAL:O       | 38:Y:57:VAL:HG12    | 2.07                     | 0.52              |
| 8:7:1:U:H6          | 8:7:1:U:H3'         | 1.74                     | 0.52              |
| 12:AB:44:VAL:HG12   | 12:AB:45:PRO:HD3    | 1.90                     | 0.52              |
| 12:AB:133:MET:SD    | 12:AB:145:ASN:C     | 2.92                     | 0.52              |
| 12:AB:144:PHE:HB3   | 12:AB:162:VAL:HG11  | 1.91                     | 0.52              |
| 10:B:76:A:N3        | 40:a:2493:U:H4'     | 2.24                     | 0.52              |
| 40:a:2298:A:C5      | 40:a:2321:U:O4      | 2.62                     | 0.52              |
| 9:9:62:ARG:HG2      | 9:9:62:ARG:NH2      | 2.20                     | 0.52              |
| 11:AA:246:LEU:HB3   | 11:AA:269:ILE:HD13  | 1.91                     | 0.52              |
| 11:AA:811:ASN:HA    | 11:AA:815:SER:HB2   | 1.90                     | 0.52              |
| 13:AC:140:ILE:HD12  | 13:AC:142:MET:HE3   | 1.92                     | 0.52              |
| 16:C:61:ARG:NH2     | 17:D:736:C:OP1      | 2.43                     | 0.52              |
| 38:Y:37:PHE:CZ      | 38:Y:56:VAL:HG11    | 2.44                     | 0.52              |
| 40:a:2315:G:O2'     | 53:n:125:ARG:HD3    | 2.09                     | 0.52              |
| 10:A:12:G:C2'       | 10:A:13:C:OP1       | 2.58                     | 0.52              |
| 10:A:17:C:O2        | 10:A:17:C:H2'       | 2.08                     | 0.52              |
| 10:A:22:G:O2'       | 10:A:23:C:P         | 2.68                     | 0.52              |
| 11:AA:524:ILE:HG21  | 11:AA:708:VAL:HG13  | 1.92                     | 0.52              |
| 11:AA:1287:LEU:HD13 | 14:AE:1357:ILE:HD11 | 1.91                     | 0.52              |
| 62:w:38:LEU:N       | 62:w:39:PRO:CD      | 2.73                     | 0.52              |
| 2:1:93:ALA:HB2      | 40:a:1614:A:N1      | 2.25                     | 0.52              |
| 4:3:94:ARG:HB3      | 4:3:103:ILE:HD12    | 1.92                     | 0.52              |
| 10:A:6:G:O2'        | 10:A:7:G:H8         | 1.92                     | 0.52              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:A:15:G:N3       | 10:A:15:G:C2'       | 2.73                     | 0.52              |
| 17:D:767:A:H2'     | 17:D:768:A:O4'      | 2.08                     | 0.52              |
| 40:a:1266:G:OP2    | 48:i:17:ARG:NE      | 2.43                     | 0.52              |
| 10:B:22:G:O2'      | 10:B:23:C:P         | 2.67                     | 0.52              |
| 38:Y:59:THR:HG22   | 38:Y:61:TYR:CE1     | 2.45                     | 0.52              |
| 53:n:8:TYR:HA      | 53:n:12:VAL:HB      | 1.91                     | 0.52              |
| 13:AD:100:LEU:HD21 | 13:AD:121:VAL:HG11  | 1.90                     | 0.52              |
| 22:I:77:ILE:HA     | 22:I:84:VAL:HG23    | 1.91                     | 0.52              |
| 65:z:58:ARG:HA     | 65:z:61:TRP:CE3     | 2.45                     | 0.52              |
| 2:1:59:GLU:HG3     | 2:1:66:ILE:HD11     | 1.92                     | 0.52              |
| 9:9:11:ILE:CD1     | 9:9:11:ILE:N        | 2.73                     | 0.52              |
| 10:A:56:C:C3'      | 10:A:57:A:H5''      | 2.40                     | 0.52              |
| 11:AA:714:VAL:HB   | 11:AA:787:PRO:HD2   | 1.92                     | 0.52              |
| 11:AA:888:THR:O    | 11:AA:913:VAL:HB    | 2.10                     | 0.52              |
| 14:AE:122:SER:HB2  | 14:AE:132:LEU:HD12  | 1.91                     | 0.52              |
| 17:D:552:U:O2'     | 31:R:83:ARG:O       | 2.27                     | 0.52              |
| 20:G:35:ARG:NH2    | 21:H:10:GLU:HG2     | 2.25                     | 0.52              |
| 24:K:81:LEU:HD13   | 24:K:123:VAL:HG12   | 1.92                     | 0.52              |
| 38:Y:33:ASN:H      | 38:Y:66:PHE:HE1     | 1.56                     | 0.52              |
| 40:a:587:C:OP2     | 60:u:21:ARG:NH1     | 2.43                     | 0.52              |
| 40:a:1693:U:O2'    | 47:h:14:ARG:NH2     | 2.43                     | 0.52              |
| 52:m:31:LEU:HD22   | 52:m:42:LEU:CD1     | 2.40                     | 0.52              |
| 8:7:11:U:C2        | 11:AA:1253:LEU:HD12 | 2.35                     | 0.52              |
| 9:9:31:ARG:HD2     | 40:a:1054:A:H5'     | 1.80                     | 0.52              |
| 11:AA:143:ARG:NH1  | 11:AA:507:GLY:O     | 2.32                     | 0.52              |
| 12:AB:133:MET:SD   | 12:AB:145:ASN:CG    | 2.92                     | 0.52              |
| 13:AD:182:ARG:NH1  | 14:AE:534:GLU:OE1   | 2.42                     | 0.52              |
| 38:Y:138:VAL:HG12  | 38:Y:138:VAL:O      | 2.08                     | 0.52              |
| 40:a:523:C:H4'     | 40:a:540:C:O2       | 2.10                     | 0.52              |
| 4:3:12:ILE:HG21    | 4:3:80:ALA:HB2      | 1.92                     | 0.52              |
| 10:A:38:A:C2'      | 10:A:39:C:H5'       | 2.39                     | 0.52              |
| 11:AA:374:GLU:HB2  | 12:AB:80:TRP:HH2    | 1.75                     | 0.52              |
| 13:AD:28:LEU:HD12  | 13:AD:201:LEU:HD23  | 1.91                     | 0.52              |
| 14:AE:67:ASP:C     | 14:AE:69:GLU:H      | 2.18                     | 0.52              |
| 14:AE:526:VAL:HG12 | 14:AE:549:LYS:HB2   | 1.90                     | 0.52              |
| 38:Y:116:MET:HE2   | 38:Y:117:THR:H      | 1.74                     | 0.52              |
| 59:t:71:ARG:NH2    | 59:t:123:LEU:O      | 2.42                     | 0.52              |
| 8:7:-6:U:OP1       | 22:I:132:ARG:NH2    | 2.43                     | 0.51              |
| 8:7:15:G:H2'       | 8:7:16:A:H8         | 1.75                     | 0.51              |
| 12:AB:161:SER:HA   | 12:AB:170:PRO:HA    | 1.91                     | 0.51              |
| 14:AE:795:TYR:OH   | 14:AE:1326:GLN:NE2  | 2.42                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:AE:959:LYS:HB3  | 14:AE:983:LYS:HB2  | 1.92                     | 0.51              |
| 10:B:6:G:O2'       | 10:B:7:G:H8        | 1.92                     | 0.51              |
| 10:B:16:C:O2       | 10:B:16:C:H2'      | 2.08                     | 0.51              |
| 10:B:18:G:C8       | 10:B:57:A:N6       | 2.70                     | 0.51              |
| 29:P:24:GLU:OE2    | 29:P:90:LEU:CD1    | 2.56                     | 0.51              |
| 33:T:40:GLN:CA     | 33:T:40:GLN:HE21   | 2.23                     | 0.51              |
| 59:t:7:MET:HE1     | 59:t:44:LYS:HD2    | 1.91                     | 0.51              |
| 12:AB:136:VAL:HG11 | 12:AB:141:PHE:HB2  | 1.92                     | 0.51              |
| 17:D:1308:U:P      | 37:X:98:ARG:HG3    | 2.50                     | 0.51              |
| 17:D:1499:A:O2'    | 17:D:1500:A:H5'    | 2.10                     | 0.51              |
| 21:H:135:LEU:CB    | 21:H:167:VAL:CA    | 2.86                     | 0.51              |
| 9:9:62:ARG:CG      | 9:9:62:ARG:NH2     | 2.73                     | 0.51              |
| 10:A:56:C:H1'      | 40:a:2112:G:C5     | 2.46                     | 0.51              |
| 11:AA:125:GLY:HA2  | 11:AA:499:SER:HB2  | 1.92                     | 0.51              |
| 12:AB:141:PHE:CZ   | 29:P:6:ILE:HD11    | 2.45                     | 0.51              |
| 14:AE:77:ARG:HB3   | 14:AE:80:HIS:HB2   | 1.93                     | 0.51              |
| 10:B:12:G:C2'      | 10:B:13:C:OP1      | 2.57                     | 0.51              |
| 40:a:118:A:C8      | 40:a:119:A:C8      | 2.99                     | 0.51              |
| 8:7:-18:G:C4'      | 17:D:1500:A:N6     | 2.73                     | 0.51              |
| 9:9:93:ALA:O       | 9:9:129:LEU:HD13   | 2.06                     | 0.51              |
| 10:A:5:G:C2'       | 10:A:6:G:H5'       | 2.40                     | 0.51              |
| 12:AB:141:PHE:HZ   | 29:P:6:ILE:HD11    | 1.75                     | 0.51              |
| 17:D:1228:C:OP1    | 37:X:107:ARG:CZ    | 2.58                     | 0.51              |
| 23:J:61:VAL:HG21   | 23:J:200:ILE:CD1   | 2.35                     | 0.51              |
| 40:a:1814:G:H4'    | 47:h:51:THR:HG21   | 1.92                     | 0.51              |
| 8:7:-19:U:H2'      | 8:7:-18:G:C8       | 2.45                     | 0.51              |
| 10:A:18:G:C2       | 10:A:58:A:C6       | 2.99                     | 0.51              |
| 11:AA:93:SER:HA    | 11:AA:128:PRO:HA   | 1.92                     | 0.51              |
| 12:AB:64:PHE:CZ    | 14:AE:285:LEU:HD21 | 2.46                     | 0.51              |
| 14:AE:71:LEU:HD22  | 14:AE:90:VAL:HG21  | 1.93                     | 0.51              |
| 15:AF:3:ARG:NH1    | 15:AF:55:GLU:OE2   | 2.40                     | 0.51              |
| 40:a:929:U:H1'     | 45:f:26:GLY:O      | 2.10                     | 0.51              |
| 8:7:-8:U:H5''      | 8:7:-8:U:C6        | 2.45                     | 0.51              |
| 8:7:16:A:H2'       | 8:7:17:G:C8        | 2.45                     | 0.51              |
| 9:9:3:LEU:HD13     | 9:9:5:LEU:H        | 1.75                     | 0.51              |
| 11:AA:903:ARG:HH12 | 29:P:90:LEU:HD11   | 1.75                     | 0.51              |
| 10:B:15:G:H22      | 10:B:20:U:H3       | 1.59                     | 0.51              |
| 16:C:30:LYS:HA     | 16:C:33:ILE:HD13   | 1.92                     | 0.51              |
| 21:H:308:GLU:O     | 21:H:310:ASP:N     | 2.43                     | 0.51              |
| 40:a:639:U:H2'     | 40:a:640:C:C6      | 2.45                     | 0.51              |
| 10:A:41:C:H4'      | 26:M:143:ARG:NH1   | 2.25                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:D:864:A:C2      | 17:D:865:A:C2      | 2.98                     | 0.51              |
| 21:H:267:TRP:CZ3   | 21:H:340:ARG:HG3   | 2.43                     | 0.51              |
| 40:a:404:A:O2'     | 40:a:405:U:OP2     | 2.22                     | 0.51              |
| 40:a:1910:G:O5'    | 40:a:1910:G:H8     | 1.93                     | 0.51              |
| 55:p:121:ILE:HD12  | 55:p:141:ILE:CG2   | 2.41                     | 0.51              |
| 2:1:24:ILE:HD13    | 2:1:36:LEU:HD11    | 1.93                     | 0.51              |
| 12:AB:47:GLU:HB3   | 12:AB:64:PHE:CD1   | 2.46                     | 0.51              |
| 12:AB:71:VAL:HG12  | 12:AB:73:MET:HB2   | 1.93                     | 0.51              |
| 14:AE:157:GLN:HE22 | 14:AE:188:LEU:HD22 | 1.76                     | 0.51              |
| 10:B:48:C:O2       | 10:B:48:C:H2'      | 2.11                     | 0.51              |
| 17:D:1404:C:H2'    | 17:D:1404:C:O2     | 2.10                     | 0.51              |
| 28:O:98:LEU:HB3    | 28:O:104:VAL:HG13  | 1.92                     | 0.51              |
| 40:a:1839:G:N9     | 40:a:1927:A:H1'    | 2.23                     | 0.51              |
| 43:d:106:G:H2'     | 43:d:107:G:O4'     | 2.10                     | 0.51              |
| 13:AD:22:THR:HG1   | 13:AD:207:THR:HG1  | 1.59                     | 0.51              |
| 21:H:19:ARG:O      | 21:H:72:LEU:HD22   | 2.09                     | 0.51              |
| 9:9:23:LEU:HA      | 9:9:118:ILE:HG13   | 1.92                     | 0.51              |
| 9:9:50:VAL:CG1     | 38:Y:119:ALA:CB    | 2.88                     | 0.51              |
| 10:A:15:G:H22      | 10:A:20:U:H3       | 1.59                     | 0.51              |
| 10:B:18:G:C2       | 10:B:58:A:C6       | 2.99                     | 0.51              |
| 38:Y:27:LEU:HD12   | 38:Y:27:LEU:C      | 2.35                     | 0.51              |
| 40:a:1406:U:H3     | 40:a:1596:A:H2     | 1.59                     | 0.51              |
| 58:s:17:VAL:HG23   | 58:s:137:PRO:HB2   | 1.93                     | 0.51              |
| 6:5:98:DA:N9       | 6:5:99:DT:H72      | 2.26                     | 0.50              |
| 9:9:31:ARG:CG      | 9:9:31:ARG:NH1     | 2.73                     | 0.50              |
| 12:AB:165:PHE:CZ   | 29:P:89:ARG:HG3    | 2.45                     | 0.50              |
| 10:B:56:C:C3'      | 10:B:57:A:H5''     | 2.40                     | 0.50              |
| 21:H:332:VAL:C     | 21:H:334:ASP:H     | 2.18                     | 0.50              |
| 40:a:1141:U:O2     | 40:a:1142:A:N6     | 2.44                     | 0.50              |
| 49:j:4:LEU:HD23    | 49:j:29:VAL:CG1    | 2.39                     | 0.50              |
| 9:9:41:LEU:HD12    | 38:Y:117:THR:HG22  | 1.92                     | 0.50              |
| 10:A:56:C:C5       | 40:a:2168:G:O6     | 2.64                     | 0.50              |
| 11:AA:562:GLU:OE1  | 11:AA:662:SER:OG   | 2.28                     | 0.50              |
| 11:AA:903:ARG:NH1  | 29:P:90:LEU:HD21   | 2.27                     | 0.50              |
| 10:B:15:G:N3       | 10:B:15:G:C2'      | 2.73                     | 0.50              |
| 10:B:47:U:H2'      | 10:B:48:C:H4'      | 1.94                     | 0.50              |
| 17:D:1410:A:C2     | 17:D:1491:G:C2     | 2.99                     | 0.50              |
| 6:5:96:DT:H2''     | 6:5:97:DC:C5       | 2.46                     | 0.50              |
| 10:A:48:C:H2'      | 10:A:48:C:O2       | 2.11                     | 0.50              |
| 10:A:76:A:O2'      | 40:a:2395:C:C2     | 2.64                     | 0.50              |
| 11:AA:400:VAL:HG21 | 11:AA:452:ARG:HE   | 1.76                     | 0.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:AA:974:ARG:HD2  | 11:AA:1014:LEU:HD21 | 1.92                     | 0.50              |
| 12:AB:123:ARG:NE   | 12:AB:123:ARG:HA    | 2.24                     | 0.50              |
| 14:AE:693:VAL:HG21 | 14:AE:743:MET:HE3   | 1.94                     | 0.50              |
| 40:a:2243:U:H2'    | 40:a:2244:U:C6      | 2.46                     | 0.50              |
| 12:AB:133:MET:CE   | 12:AB:163:SER:CB    | 2.89                     | 0.50              |
| 12:AB:144:PHE:HE1  | 29:P:85:ASP:OD2     | 1.86                     | 0.50              |
| 10:B:34:C:O2       | 10:B:34:C:H2'       | 2.11                     | 0.50              |
| 17:D:1276:G:O5'    | 17:D:1276:G:H8      | 1.93                     | 0.50              |
| 21:H:117:LYS:CB    | 21:H:278:THR:CG2    | 2.90                     | 0.50              |
| 40:a:1824:G:O2'    | 47:h:252:THR:HG21   | 2.11                     | 0.50              |
| 14:AE:679:TYR:OH   | 14:AE:754:ILE:O     | 2.23                     | 0.50              |
| 10:B:24:U:O2'      | 40:a:1922:G:O3'     | 2.29                     | 0.50              |
| 17:D:1499:A:H3'    | 17:D:1499:A:OP2     | 2.12                     | 0.50              |
| 29:P:57:VAL:O      | 29:P:57:VAL:HG13    | 2.11                     | 0.50              |
| 38:Y:112:LYS:NZ    | 38:Y:112:LYS:CB     | 2.73                     | 0.50              |
| 40:a:2297:A:C6     | 40:a:2321:U:O4      | 2.65                     | 0.50              |
| 12:AB:169:THR:HG21 | 29:P:84:VAL:CG1     | 2.38                     | 0.50              |
| 14:AE:417:ARG:NH1  | 15:AF:43:ASN:O      | 2.45                     | 0.50              |
| 14:AE:1179:PRO:HB2 | 14:AE:1182:GLY:H    | 1.75                     | 0.50              |
| 40:a:1869:G:N2     | 40:a:1871:A:O2'     | 2.44                     | 0.50              |
| 8:7:-10:U:O2'      | 24:K:33:PHE:CZ      | 2.52                     | 0.50              |
| 10:A:76:A:C2'      | 40:a:2394:C:N4      | 2.75                     | 0.50              |
| 14:AE:209:ASN:HB3  | 14:AE:214:ARG:HH21  | 1.76                     | 0.50              |
| 14:AE:640:GLY:N    | 14:AE:643:ASP:OD2   | 2.42                     | 0.50              |
| 21:H:49:PRO:HD2    | 21:H:84:LEU:HD11    | 1.92                     | 0.50              |
| 59:t:113:MET:O     | 59:t:116:ILE:HG13   | 2.11                     | 0.50              |
| 11:AA:232:ILE:HG12 | 11:AA:237:LEU:HG    | 1.93                     | 0.50              |
| 11:AA:845:LEU:HD21 | 11:AA:890:LYS:C     | 2.37                     | 0.50              |
| 12:AB:148:VAL:CG2  | 12:AB:151:VAL:HG23  | 2.41                     | 0.50              |
| 17:D:108:G:H5''    | 17:D:108:G:N3       | 2.27                     | 0.50              |
| 17:D:1356:G:H2'    | 17:D:1357:A:C8      | 2.47                     | 0.50              |
| 40:a:464:U:O3'     | 52:m:12:ARG:NH2     | 2.45                     | 0.50              |
| 40:a:2298:A:N3     | 40:a:2321:U:C5      | 2.80                     | 0.50              |
| 49:j:25:THR:HG21   | 49:j:193:VAL:HG22   | 1.94                     | 0.50              |
| 59:t:43:ILE:HD12   | 59:t:56:ASP:HB2     | 1.93                     | 0.50              |
| 8:7:-19:U:OP2      | 17:D:926:G:N2       | 2.45                     | 0.50              |
| 11:AA:411:ARG:NH2  | 11:AA:427:ASP:OD2   | 2.44                     | 0.50              |
| 10:B:25:C:H2'      | 10:B:26:G:H5'       | 1.94                     | 0.50              |
| 27:N:3:MET:HA      | 27:N:3:MET:HE3      | 1.94                     | 0.50              |
| 33:T:21:ASP:O      | 33:T:22:THR:HG22    | 2.12                     | 0.50              |
| 40:a:560:C:O2      | 65:z:48:ARG:NH1     | 2.41                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AA:18:ARG:HE    | 11:AA:620:ASN:HA   | 1.77                     | 0.49              |
| 10:B:72:A:H2'      | 10:B:73:A:C5'      | 2.33                     | 0.49              |
| 17:D:872:A:H2'     | 17:D:872:A:N3      | 2.27                     | 0.49              |
| 17:D:1366:C:O2'    | 29:P:62:ARG:NH2    | 2.44                     | 0.49              |
| 33:T:4:SER:O       | 33:T:8:THR:HG23    | 2.12                     | 0.49              |
| 38:Y:100:ILE:HB    | 38:Y:105:LEU:HD11  | 1.92                     | 0.49              |
| 40:a:742:A:C2      | 40:a:743:A:C6      | 3.00                     | 0.49              |
| 1:O:14:VAL:HG21    | 1:O:98:ILE:HG13    | 1.94                     | 0.49              |
| 11:AA:1340:GLU:HB2 | 14:AE:19:ALA:HB3   | 1.94                     | 0.49              |
| 13:AD:100:LEU:HB2  | 13:AD:144:ILE:HG23 | 1.95                     | 0.49              |
| 14:AE:425:ARG:NH1  | 14:AE:458:ASN:O    | 2.45                     | 0.49              |
| 14:AE:430:HIS:HB3  | 14:AE:925:GLU:HG3  | 1.93                     | 0.49              |
| 24:K:114:VAL:HG21  | 24:K:141:ILE:HD12  | 1.94                     | 0.49              |
| 47:h:107:PRO:HD2   | 47:h:110:LEU:HD22  | 1.94                     | 0.49              |
| 10:A:28:C:H2'      | 10:A:29:G:H8       | 1.76                     | 0.49              |
| 10:B:60:U:O2'      | 10:B:61:C:OP1      | 2.23                     | 0.49              |
| 17:D:1208:C:H2'    | 17:D:1209:C:C6     | 2.47                     | 0.49              |
| 11:AA:400:VAL:HG11 | 11:AA:452:ARG:HD2  | 1.94                     | 0.49              |
| 11:AA:529:ARG:HH11 | 11:AA:572:ILE:HG22 | 1.77                     | 0.49              |
| 12:AB:173:LEU:HB3  | 12:AB:178:VAL:HG13 | 1.94                     | 0.49              |
| 14:AE:107:LEU:HD22 | 14:AE:299:LEU:HD21 | 1.94                     | 0.49              |
| 10:B:59:A:H2'      | 10:B:60:U:H5'      | 1.94                     | 0.49              |
| 17:D:50:A:O2'      | 17:D:360:G:N2      | 2.45                     | 0.49              |
| 17:D:1311:A:OP1    | 46:g:59:ARG:NH1    | 2.45                     | 0.49              |
| 40:a:2646:C:O5'    | 40:a:2646:C:H6     | 1.95                     | 0.49              |
| 55:p:35:ARG:HD3    | 55:p:71:LEU:HD13   | 1.94                     | 0.49              |
| 8:7:-15:U:C2       | 17:D:1493:A:C2     | 3.00                     | 0.49              |
| 9:9:51:TYR:CG      | 9:9:89:PRO:HD2     | 2.47                     | 0.49              |
| 9:9:125:ARG:HG3    | 9:9:125:ARG:O      | 2.10                     | 0.49              |
| 12:AB:144:PHE:HE2  | 29:P:81:GLU:HA     | 1.77                     | 0.49              |
| 10:B:42:G:H2'      | 10:B:43:A:C8       | 2.48                     | 0.49              |
| 17:D:1169:A:H2'    | 17:D:1170:A:C8     | 2.48                     | 0.49              |
| 21:H:318:PRO:HA    | 21:H:321:VAL:HG12  | 1.95                     | 0.49              |
| 40:a:1964:G:H4'    | 40:a:1965:C:OP2    | 2.11                     | 0.49              |
| 41:b:37:ILE:HG21   | 41:b:80:ILE:HG21   | 1.95                     | 0.49              |
| 8:7:-15:U:C2       | 17:D:1493:A:H2     | 2.31                     | 0.49              |
| 8:7:12:G:C4        | 14:AE:253:VAL:HG21 | 2.47                     | 0.49              |
| 9:9:44:ALA:HB1     | 9:9:52:MET:HB3     | 1.93                     | 0.49              |
| 11:AA:255:ILE:HB   | 11:AA:263:VAL:HB   | 1.92                     | 0.49              |
| 11:AA:732:ILE:HD11 | 11:AA:769:PRO:HB3  | 1.95                     | 0.49              |
| 11:AA:910:ALA:HB1  | 11:AA:913:VAL:HG12 | 1.93                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:AB:144:PHE:HE1  | 29:P:85:ASP:CG      | 2.20                     | 0.49              |
| 14:AE:814:CYS:SG   | 14:AE:815:GLY:N     | 2.85                     | 0.49              |
| 19:F:4:ILE:HD12    | 19:F:19:PHE:HA      | 1.93                     | 0.49              |
| 21:H:132:PRO:N     | 21:H:167:VAL:CB     | 2.75                     | 0.49              |
| 35:V:48:ASP:HB3    | 35:V:75:LEU:HD23    | 1.94                     | 0.49              |
| 40:a:2038:G:H2'    | 40:a:2039:U:O4'     | 2.13                     | 0.49              |
| 45:f:24:LEU:HD11   | 45:f:54:MET:CE      | 2.42                     | 0.49              |
| 2:1:55:ILE:HG23    | 2:1:66:ILE:HD12     | 1.93                     | 0.49              |
| 10:A:18:G:C5       | 10:A:57:A:C5        | 3.01                     | 0.49              |
| 12:AB:136:VAL:HG22 | 12:AB:173:LEU:CD1   | 2.42                     | 0.49              |
| 10:B:18:G:C5       | 10:B:57:A:C5        | 3.01                     | 0.49              |
| 40:a:1412:U:C4     | 40:a:1413:A:N7      | 2.81                     | 0.49              |
| 47:h:210:ALA:HA    | 47:h:213:TRP:CE3    | 2.48                     | 0.49              |
| 53:n:127:ASN:ND2   | 53:n:127:ASN:N      | 2.60                     | 0.49              |
| 58:s:30:THR:HG22   | 58:s:31:GLU:N       | 2.27                     | 0.49              |
| 9:9:31:ARG:NE      | 40:a:1054:A:O4'     | 2.46                     | 0.49              |
| 10:A:37:A:H2'      | 10:A:38:A:H8        | 1.77                     | 0.49              |
| 14:AE:429:LEU:HB3  | 14:AE:925:GLU:HG2   | 1.95                     | 0.49              |
| 38:Y:80:LYS:HG3    | 38:Y:86:LYS:HA      | 1.93                     | 0.49              |
| 40:a:1433:A:H2'    | 40:a:1434:A:O4'     | 2.13                     | 0.49              |
| 58:s:32:LEU:CD2    | 58:s:54:ILE:HG21    | 2.42                     | 0.49              |
| 8:7:-13:U:OP2      | 17:D:1397:C:C2      | 2.65                     | 0.49              |
| 14:AE:412:LEU:HD22 | 14:AE:441:LEU:HD21  | 1.94                     | 0.49              |
| 10:B:15:G:C2       | 10:B:20:U:O2        | 2.66                     | 0.49              |
| 20:G:35:ARG:CD     | 21:H:14:LYS:HD3     | 2.40                     | 0.49              |
| 29:P:6:ILE:HG23    | 29:P:100:ILE:CG2    | 2.43                     | 0.49              |
| 40:a:2557:G:H2'    | 40:a:2558:C:C6      | 2.47                     | 0.49              |
| 6:5:108:DT:H73     | 11:AA:199:ASP:HB3   | 1.95                     | 0.49              |
| 14:AE:67:ASP:C     | 14:AE:69:GLU:N      | 2.71                     | 0.49              |
| 10:B:39:C:O5'      | 10:B:39:C:H6        | 1.95                     | 0.49              |
| 62:w:55:ALA:HA     | 62:w:80:PHE:CE1     | 2.47                     | 0.49              |
| 2:1:4:ILE:HG12     | 2:1:106:VAL:HG22    | 1.95                     | 0.48              |
| 7:6:16:DC:H1'      | 14:AE:426:ALA:HB1   | 1.95                     | 0.48              |
| 11:AA:9:LYS:HG2    | 11:AA:1171:ARG:HH12 | 1.77                     | 0.48              |
| 11:AA:146:VAL:HG21 | 11:AA:513:GLN:HE21  | 1.77                     | 0.48              |
| 11:AA:554:HIS:HD2  | 11:AA:558:VAL:HB    | 1.77                     | 0.48              |
| 12:AB:133:MET:SD   | 12:AB:145:ASN:HB2   | 2.53                     | 0.48              |
| 10:B:5:G:C2'       | 10:B:6:G:H5'        | 2.40                     | 0.48              |
| 10:B:11:A:H2'      | 10:B:12:G:C1'       | 2.43                     | 0.48              |
| 21:H:120:PHE:CB    | 21:H:136:VAL:CB     | 2.91                     | 0.48              |
| 17:D:5:U:O2        | 17:D:5:U:O4'        | 2.29                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:L:18:VAL:N      | 25:L:19:PRO:CD      | 2.76                     | 0.48              |
| 65:z:47:TYR:CD1    | 65:z:47:TYR:C       | 2.90                     | 0.48              |
| 2:1:25:ARG:NH1     | 2:1:74:ILE:O        | 2.46                     | 0.48              |
| 4:3:7:ARG:HB2      | 40:a:85:G:OP2       | 2.13                     | 0.48              |
| 10:A:59:A:H2'      | 10:A:60:U:H5'       | 1.94                     | 0.48              |
| 11:AA:1314:GLN:HB2 | 15:AF:28:ARG:HH12   | 1.79                     | 0.48              |
| 12:AB:48:GLU:HB3   | 12:AB:62:ARG:CG     | 2.43                     | 0.48              |
| 12:AB:151:VAL:HG13 | 12:AB:158:LEU:HD23  | 1.95                     | 0.48              |
| 17:D:974:A:OP1     | 32:S:69:ARG:NH1     | 2.46                     | 0.48              |
| 40:a:2303:G:C6     | 40:a:2314:A:N1      | 2.81                     | 0.48              |
| 62:w:67:PHE:O      | 62:w:71:ARG:N       | 2.45                     | 0.48              |
| 9:9:31:ARG:HE      | 40:a:1054:A:C4'     | 2.26                     | 0.48              |
| 10:A:11:A:H2'      | 10:A:12:G:C1'       | 2.42                     | 0.48              |
| 10:A:25:C:H2'      | 10:A:26:G:H5'       | 1.95                     | 0.48              |
| 10:A:42:G:H2'      | 10:A:43:A:C8        | 2.47                     | 0.48              |
| 10:A:76:A:N6       | 40:a:2422:C:O4'     | 2.46                     | 0.48              |
| 11:AA:618:GLN:HG3  | 14:AE:770:LEU:HD13  | 1.95                     | 0.48              |
| 11:AA:896:THR:H    | 11:AA:899:GLU:HB2   | 1.78                     | 0.48              |
| 21:H:23:ILE:N      | 21:H:69:ASP:OD2     | 2.47                     | 0.48              |
| 29:P:6:ILE:CG2     | 29:P:100:ILE:HG23   | 2.43                     | 0.48              |
| 38:Y:77:VAL:HG13   | 38:Y:80:LYS:HE3     | 1.95                     | 0.48              |
| 42:c:3:ARG:HD2     | 42:c:30:LEU:HD22    | 1.95                     | 0.48              |
| 9:9:8:LYS:NZ       | 40:a:1046:A:H61     | 2.11                     | 0.48              |
| 9:9:125:ARG:NH1    | 9:9:125:ARG:CA      | 2.73                     | 0.48              |
| 14:AE:749:LYS:HD3  | 14:AE:753:SER:HB2   | 1.94                     | 0.48              |
| 21:H:330:VAL:HG12  | 21:H:345:GLY:O      | 2.14                     | 0.48              |
| 24:K:99:ALA:CB     | 24:K:103:THR:HG21   | 2.43                     | 0.48              |
| 40:a:2303:G:C2     | 40:a:2314:A:N3      | 2.82                     | 0.48              |
| 40:a:2685:G:OP1    | 59:t:78:ARG:NH2     | 2.47                     | 0.48              |
| 49:j:156:PHE:CE1   | 58:s:81:ILE:HD13    | 2.48                     | 0.48              |
| 52:m:24:THR:HG23   | 52:m:27:GLY:H       | 1.78                     | 0.48              |
| 9:9:23:LEU:HD22    | 9:9:92:ALA:HB1      | 1.95                     | 0.48              |
| 10:A:47:U:H2'      | 10:A:48:C:H4'       | 1.94                     | 0.48              |
| 11:AA:836:LEU:HD13 | 11:AA:1054:LEU:HD13 | 1.95                     | 0.48              |
| 10:B:49:G:O5'      | 10:B:49:G:H8        | 1.96                     | 0.48              |
| 17:D:13:U:O4       | 17:D:21:G:N3        | 2.46                     | 0.48              |
| 17:D:1308:U:H2'    | 37:X:98:ARG:HH22    | 1.61                     | 0.48              |
| 40:a:565:C:H2'     | 40:a:566:U:O4'      | 2.13                     | 0.48              |
| 8:7:12:G:N3        | 14:AE:253:VAL:HG21  | 2.29                     | 0.48              |
| 10:A:58:A:OP2      | 10:A:58:A:C8        | 2.67                     | 0.48              |
| 12:AB:65:PHE:HZ    | 12:AB:70:LEU:CD1    | 2.11                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:Y:77:VAL:HG13   | 38:Y:80:LYS:CE     | 2.44                     | 0.48              |
| 63:x:51:ALA:HB3    | 63:x:78:VAL:HB     | 1.94                     | 0.48              |
| 10:A:41:C:H5'      | 26:M:143:ARG:HD2   | 1.95                     | 0.48              |
| 11:AA:1311:GLY:O   | 15:AF:31:GLN:NE2   | 2.47                     | 0.48              |
| 12:AB:174:ASP:O    | 12:AB:178:VAL:HG22 | 2.14                     | 0.48              |
| 13:AC:102:LEU:HD12 | 13:AC:115:ILE:HG12 | 1.96                     | 0.48              |
| 17:D:911:U:H2'     | 17:D:912:C:C6      | 2.49                     | 0.48              |
| 54:o:13:ARG:HD3    | 60:u:58:TYR:O      | 2.14                     | 0.48              |
| 57:r:3:VAL:HG22    | 57:r:36:ALA:HB1    | 1.95                     | 0.48              |
| 1:0:14:VAL:CG2     | 1:0:98:ILE:HG13    | 2.43                     | 0.48              |
| 8:7:-13:U:H5'      | 17:D:1397:C:C2     | 2.48                     | 0.48              |
| 9:9:51:TYR:CD1     | 9:9:88:HIS:HB2     | 2.49                     | 0.48              |
| 9:9:52:MET:HE3     | 9:9:52:MET:CA      | 2.42                     | 0.48              |
| 14:AE:678:ARG:NH1  | 14:AE:756:GLU:OE1  | 2.46                     | 0.48              |
| 17:D:13:U:O2       | 17:D:915:A:N7      | 2.47                     | 0.48              |
| 40:a:742:A:C2      | 40:a:755:U:N3      | 2.81                     | 0.48              |
| 40:a:1209:U:O2'    | 40:a:1237:A:N1     | 2.40                     | 0.48              |
| 40:a:1588:G:C6     | 40:a:1589:U:O4     | 2.67                     | 0.48              |
| 40:a:1980:G:O2'    | 40:a:1982:U:OP2    | 2.28                     | 0.48              |
| 10:A:49:G:H8       | 10:A:49:G:O5'      | 1.96                     | 0.48              |
| 11:AA:318:SER:OG   | 11:AA:320:ASP:OD1  | 2.31                     | 0.48              |
| 14:AE:520:ALA:HB3  | 14:AE:546:ALA:HB2  | 1.95                     | 0.48              |
| 14:AE:1289:ASN:ND2 | 14:AE:1300:ALA:O   | 2.46                     | 0.48              |
| 10:B:18:G:N3       | 10:B:58:A:C6       | 2.82                     | 0.48              |
| 10:B:68:C:C4       | 10:B:69:C:C5       | 3.02                     | 0.48              |
| 17:D:371:A:H2'     | 17:D:372:C:O4'     | 2.14                     | 0.48              |
| 40:a:1814:G:C4'    | 47:h:51:THR:HG21   | 2.44                     | 0.48              |
| 40:a:2168:G:H8     | 40:a:2168:G:OP1    | 1.97                     | 0.48              |
| 49:j:121:THR:HB    | 49:j:127:PHE:CD2   | 2.49                     | 0.48              |
| 52:m:22:MET:O      | 52:m:28:ARG:NH1    | 2.45                     | 0.48              |
| 2:1:29:VAL:HB      | 2:1:55:ILE:HD11    | 1.95                     | 0.47              |
| 8:7:16:A:H2'       | 8:7:17:G:H8        | 1.79                     | 0.47              |
| 10:A:11:A:C2'      | 10:A:12:G:O4'      | 2.60                     | 0.47              |
| 10:A:15:G:C2       | 10:A:20:U:O2       | 2.66                     | 0.47              |
| 14:AE:616:PRO:HA   | 14:AE:619:ILE:HG22 | 1.96                     | 0.47              |
| 14:AE:804:ALA:O    | 14:AE:806:ASP:N    | 2.47                     | 0.47              |
| 17:D:1017:U:O2'    | 17:D:1018:G:O4'    | 2.31                     | 0.47              |
| 40:a:1993:U:H4'    | 49:j:133:THR:HG22  | 1.96                     | 0.47              |
| 44:e:18:LEU:HB2    | 44:e:53:VAL:HG11   | 1.95                     | 0.47              |
| 63:x:27:VAL:CG2    | 63:x:40:ILE:HD12   | 2.44                     | 0.47              |
| 1:0:40:MET:HE3     | 1:0:49:ILE:CD1     | 2.44                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:2:61:LEU:C        | 3:2:61:LEU:HD12     | 2.39                     | 0.47              |
| 10:A:37:A:H2'       | 10:A:38:A:C8        | 2.48                     | 0.47              |
| 10:A:60:U:H4'       | 10:A:61:C:OP2       | 2.14                     | 0.47              |
| 10:A:68:C:C4        | 10:A:69:C:C5        | 3.02                     | 0.47              |
| 12:AB:128:PHE:CE1   | 12:AB:180:LYS:HD2   | 2.49                     | 0.47              |
| 12:AB:140:PRO:HB2   | 29:P:80:THR:O       | 2.14                     | 0.47              |
| 14:AE:218:THR:HA    | 14:AE:221:ILE:HG22  | 1.96                     | 0.47              |
| 10:B:9:G:H5''       | 10:B:10:G:OP2       | 2.14                     | 0.47              |
| 17:D:35:G:N3        | 31:R:115:SER:OG     | 2.47                     | 0.47              |
| 7:6:21:DA:N6        | 8:7:15:G:N1         | 2.61                     | 0.47              |
| 8:7:-2:U:O2         | 8:7:-2:U:H2'        | 2.12                     | 0.47              |
| 8:7:14:U:H5''       | 14:AE:322:ARG:HD2   | 1.95                     | 0.47              |
| 10:A:14:A:H2'       | 10:A:14:A:N3        | 2.29                     | 0.47              |
| 10:A:18:G:N3        | 10:A:58:A:C6        | 2.82                     | 0.47              |
| 10:A:33:U:H2'       | 10:A:35:A:OP2       | 2.14                     | 0.47              |
| 11:AA:812:PHE:O     | 14:AE:504:GLN:NE2   | 2.40                     | 0.47              |
| 12:AB:168:ALA:CB    | 29:P:88:MET:CA      | 2.88                     | 0.47              |
| 14:AE:1108:GLN:HE21 | 14:AE:1123:ARG:HH12 | 1.62                     | 0.47              |
| 14:AE:1350:ASN:HA   | 14:AE:1353:VAL:HG12 | 1.97                     | 0.47              |
| 10:B:11:A:C2'       | 10:B:12:G:O4'       | 2.60                     | 0.47              |
| 35:V:75:LEU:C       | 35:V:75:LEU:HD12    | 2.38                     | 0.47              |
| 40:a:2093:G:O2'     | 40:a:2198:A:N1      | 2.41                     | 0.47              |
| 9:9:17:GLU:HG2      | 9:9:88:HIS:NE2      | 2.29                     | 0.47              |
| 10:A:9:G:H5''       | 10:A:10:G:OP2       | 2.14                     | 0.47              |
| 11:AA:363:LEU:HB3   | 11:AA:381:ALA:HB1   | 1.96                     | 0.47              |
| 11:AA:565:GLU:HA    | 11:AA:569:ILE:HG12  | 1.95                     | 0.47              |
| 11:AA:848:GLU:HG2   | 11:AA:888:THR:HG22  | 1.96                     | 0.47              |
| 12:AB:171:VAL:HG21  | 29:P:102:LEU:CG     | 2.45                     | 0.47              |
| 17:D:604:G:H2'      | 17:D:605:U:O4'      | 2.14                     | 0.47              |
| 17:D:1174:G:H2'     | 17:D:1175:G:H5'     | 1.95                     | 0.47              |
| 40:a:686:U:O4       | 52:m:12:ARG:HB2     | 2.14                     | 0.47              |
| 10:B:14:A:N3        | 10:B:14:A:H2'       | 2.29                     | 0.47              |
| 10:B:58:A:C8        | 10:B:58:A:OP2       | 2.67                     | 0.47              |
| 10:B:76:A:N3        | 10:B:76:A:C2'       | 2.74                     | 0.47              |
| 16:C:12:ARG:NH2     | 21:H:268:VAL:CG2    | 2.71                     | 0.47              |
| 58:s:84:ILE:HG23    | 58:s:84:ILE:O       | 2.14                     | 0.47              |
| 8:7:-14:U:C6        | 8:7:-14:U:C3'       | 2.97                     | 0.47              |
| 10:A:18:G:C6        | 10:A:57:A:N7        | 2.83                     | 0.47              |
| 11:AA:689:ALA:HB2   | 11:AA:1233:LEU:HD23 | 1.97                     | 0.47              |
| 11:AA:1286:THR:O    | 11:AA:1290:MET:HB2  | 2.14                     | 0.47              |
| 12:AB:171:VAL:HG21  | 29:P:102:LEU:CD2    | 2.44                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:AE:977:SER:OG   | 14:AE:980:THR:OG1  | 2.31                     | 0.47              |
| 17:D:1064:G:O2'    | 17:D:1190:G:N2     | 2.47                     | 0.47              |
| 17:D:1329:A:OP1    | 37:X:28:THR:OG1    | 2.31                     | 0.47              |
| 21:H:309:MET:HE2   | 21:H:318:PRO:HB3   | 1.97                     | 0.47              |
| 27:N:102:ALA:HB3   | 27:N:113:ASP:HB3   | 1.96                     | 0.47              |
| 9:9:27:VAL:HG22    | 9:9:99:PHE:HE2     | 1.80                     | 0.47              |
| 9:9:57:ASN:CG      | 9:9:62:ARG:HG3     | 2.30                     | 0.47              |
| 9:9:67:THR:H       | 9:9:68:PRO:HD3     | 1.80                     | 0.47              |
| 11:AA:1280:ALA:HB1 | 14:AE:918:ILE:HG22 | 1.96                     | 0.47              |
| 13:AD:182:ARG:O    | 13:AD:205:MET:HA   | 2.14                     | 0.47              |
| 14:AE:66:LYS:HB2   | 14:AE:69:GLU:HB3   | 1.96                     | 0.47              |
| 14:AE:77:ARG:HA    | 14:AE:77:ARG:CZ    | 2.44                     | 0.47              |
| 14:AE:86:GLU:N     | 14:AE:86:GLU:CD    | 2.73                     | 0.47              |
| 14:AE:437:PHE:HZ   | 14:AE:453:VAL:HG11 | 1.79                     | 0.47              |
| 10:B:18:G:C6       | 10:B:57:A:N7       | 2.83                     | 0.47              |
| 17:D:526:C:P       | 31:R:88:LYS:HE3    | 2.54                     | 0.47              |
| 21:H:84:LEU:N      | 21:H:84:LEU:CD2    | 2.78                     | 0.47              |
| 38:Y:133:ARG:O     | 38:Y:133:ARG:HG2   | 2.14                     | 0.47              |
| 40:a:1839:G:N9     | 40:a:1927:A:C1'    | 2.77                     | 0.47              |
| 43:d:5:U:OP1       | 43:d:61:G:O2'      | 2.26                     | 0.47              |
| 11:AA:400:VAL:HG22 | 11:AA:584:TYR:HB3  | 1.96                     | 0.47              |
| 11:AA:560:PRO:O    | 14:AE:780:ARG:NH2  | 2.47                     | 0.47              |
| 12:AB:128:PHE:CE1  | 12:AB:180:LYS:CB   | 2.96                     | 0.47              |
| 23:J:162:ALA:O     | 23:J:165:ARG:O     | 2.33                     | 0.47              |
| 24:K:111:MET:CE    | 24:K:125:ALA:HB1   | 2.39                     | 0.47              |
| 59:t:18:ARG:HB2    | 59:t:45:GLU:HB3    | 1.97                     | 0.47              |
| 4:3:94:ARG:CB      | 4:3:103:ILE:HD12   | 2.45                     | 0.47              |
| 6:5:108:DT:O4      | 11:AA:199:ASP:OD2  | 2.33                     | 0.47              |
| 8:7:14:U:O4'       | 14:AE:322:ARG:NH1  | 2.48                     | 0.47              |
| 9:9:1:MET:SD       | 9:9:2:ALA:N        | 2.88                     | 0.47              |
| 9:9:31:ARG:HD3     | 40:a:1054:A:H4'    | 1.96                     | 0.47              |
| 11:AA:207:THR:OG1  | 11:AA:354:ASP:OD2  | 2.32                     | 0.47              |
| 14:AE:47:ARG:HG2   | 29:P:81:GLU:OE1    | 2.14                     | 0.47              |
| 10:B:5:G:C2'       | 10:B:6:G:C5'       | 2.93                     | 0.47              |
| 17:D:13:U:C4       | 17:D:915:A:C6      | 2.92                     | 0.47              |
| 17:D:1308:U:P      | 37:X:98:ARG:CG     | 3.03                     | 0.47              |
| 39:Z:4:LYS:O       | 39:Z:4:LYS:HD2     | 2.15                     | 0.47              |
| 55:p:24:ILE:CD1    | 55:p:72:LEU:HD21   | 2.44                     | 0.47              |
| 9:9:118:ILE:HB     | 9:9:119:PRO:CD     | 2.45                     | 0.47              |
| 10:A:29:G:H2'      | 10:A:30:G:O4'      | 2.15                     | 0.47              |
| 13:AC:64:VAL:HG11  | 13:AC:78:ILE:HG21  | 1.97                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:AE:1037:PHE:HB3 | 14:AE:1040:MET:HB2 | 1.97                     | 0.47              |
| 10:B:60:U:H4'      | 10:B:61:C:OP2      | 2.14                     | 0.47              |
| 22:I:75:ILE:HD13   | 22:I:75:ILE:C      | 2.40                     | 0.47              |
| 38:Y:21:PRO:CB     | 38:Y:22:PRO:CD     | 2.90                     | 0.47              |
| 1:O:5:PHE:HB3      | 1:O:59:ILE:HD12    | 1.96                     | 0.46              |
| 11:AA:28:LEU:HD21  | 11:AA:524:ILE:HG13 | 1.97                     | 0.46              |
| 12:AB:135:ARG:O    | 12:AB:178:VAL:HA   | 2.15                     | 0.46              |
| 21:H:291:GLY:HA2   | 21:H:305:HIS:O     | 2.15                     | 0.46              |
| 24:K:96:MET:CE     | 24:K:115:LEU:HD11  | 2.46                     | 0.46              |
| 38:Y:71:LYS:HB3    | 38:Y:72:THR:H      | 1.58                     | 0.46              |
| 39:Z:18:ASP:HB3    | 39:Z:22:LEU:CD1    | 2.45                     | 0.46              |
| 40:a:2168:G:OP1    | 40:a:2168:G:C8     | 2.68                     | 0.46              |
| 49:j:152:PRO:HG3   | 49:j:156:PHE:CZ    | 2.50                     | 0.46              |
| 14:AE:797:THR:HG22 | 14:AE:924:GLY:HA3  | 1.97                     | 0.46              |
| 10:B:18:G:C8       | 10:B:57:A:N1       | 2.83                     | 0.46              |
| 17:D:1103:C:O2     | 20:G:106:THR:HG21  | 2.15                     | 0.46              |
| 17:D:1175:G:N3     | 17:D:1176:A:C8     | 2.83                     | 0.46              |
| 17:D:1228:C:P      | 37:X:107:ARG:HH12  | 2.38                     | 0.46              |
| 40:a:1020:A:C6     | 40:a:1141:U:O2     | 2.68                     | 0.46              |
| 9:9:24:SER:HB2     | 9:9:116:GLU:HG2    | 1.97                     | 0.46              |
| 9:9:132:TYR:CE1    | 39:Z:19:VAL:HG22   | 2.50                     | 0.46              |
| 11:AA:909:LYS:HG2  | 29:P:31:ARG:HD2    | 1.98                     | 0.46              |
| 12:AB:52:ILE:HG22  | 12:AB:53:ARG:HG3   | 1.97                     | 0.46              |
| 13:AD:15:ASP:OD1   | 13:AD:27:THR:OG1   | 2.30                     | 0.46              |
| 40:a:2585:U:O2     | 40:a:2585:U:O4'    | 2.32                     | 0.46              |
| 40:a:2756:U:C4     | 40:a:2759:G:C6     | 3.03                     | 0.46              |
| 11:AA:176:ILE:HD11 | 11:AA:428:VAL:HG21 | 1.98                     | 0.46              |
| 12:AB:138:ASP:OD1  | 12:AB:139:GLY:N    | 2.49                     | 0.46              |
| 12:AB:164:ILE:O    | 12:AB:164:ILE:HG12 | 2.10                     | 0.46              |
| 17:D:373:A:C2      | 17:D:374:A:C8      | 3.03                     | 0.46              |
| 17:D:915:A:C8      | 17:D:915:A:H3'     | 2.50                     | 0.46              |
| 25:L:67:PRO:O      | 25:L:70:VAL:HG22   | 2.15                     | 0.46              |
| 40:a:2636:C:HO2'   | 49:j:45:TYR:HH     | 1.59                     | 0.46              |
| 10:A:18:G:C8       | 10:A:57:A:N1       | 2.83                     | 0.46              |
| 12:AB:57:ARG:HB3   | 12:AB:58:ARG:H     | 1.61                     | 0.46              |
| 17:D:946:A:H2'     | 17:D:947:G:C8      | 2.50                     | 0.46              |
| 21:H:52:GLN:O      | 21:H:53:PHE:HD1    | 1.95                     | 0.46              |
| 30:Q:34:ILE:HG12   | 30:Q:70:CYS:SG     | 2.56                     | 0.46              |
| 40:a:517:C:OP2     | 48:i:10:ARG:NH2    | 2.48                     | 0.46              |
| 40:a:784:G:H5'     | 40:a:785:G:OP1     | 2.16                     | 0.46              |
| 40:a:2315:G:H5'    | 53:n:157:THR:HG23  | 1.97                     | 0.46              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 61:v:96:ILE:HG21    | 61:v:126:ILE:HD12  | 1.97                     | 0.46              |
| 3:2:30:ILE:HD13     | 3:2:93:LEU:HD12    | 1.97                     | 0.46              |
| 9:9:48:ALA:HB3      | 9:9:51:TYR:CD2     | 2.50                     | 0.46              |
| 9:9:60:LEU:HB2      | 9:9:61:ARG:NH2     | 2.31                     | 0.46              |
| 10:A:68:C:H3'       | 10:A:69:C:H5''     | 1.96                     | 0.46              |
| 11:AA:812:PHE:HZ    | 14:AE:503:SER:HB2  | 1.80                     | 0.46              |
| 12:AB:133:MET:CG    | 12:AB:163:SER:OG   | 2.41                     | 0.46              |
| 14:AE:781:LYS:HD2   | 14:AE:933:ARG:HH12 | 1.81                     | 0.46              |
| 10:B:6:G:O2'        | 10:B:7:G:C5'       | 2.64                     | 0.46              |
| 10:B:48:C:N4        | 10:B:59:A:C5       | 2.84                     | 0.46              |
| 16:C:61:ARG:HG2     | 25:L:88:MET:HE1    | 1.98                     | 0.46              |
| 21:H:332:VAL:HG13   | 21:H:342:ILE:HG23  | 1.98                     | 0.46              |
| 29:P:28:THR:HG21    | 29:P:87:LEU:CD1    | 2.46                     | 0.46              |
| 40:a:1695:G:N7      | 47:h:14:ARG:NH2    | 2.64                     | 0.46              |
| 7:6:18:DC:C2        | 8:7:17:G:N2        | 2.78                     | 0.46              |
| 9:9:39:THR:HA       | 9:9:42:ARG:HH11    | 1.81                     | 0.46              |
| 9:9:58:THR:HB       | 9:9:82:ILE:H       | 1.80                     | 0.46              |
| 10:A:32:C:O2'       | 26:M:86:GLN:CD     | 2.31                     | 0.46              |
| 11:AA:1002:LEU:HD21 | 11:AA:1007:LYS:HB2 | 1.98                     | 0.46              |
| 13:AD:212:ASP:OD1   | 13:AD:212:ASP:N    | 2.48                     | 0.46              |
| 10:B:14:A:H1'       | 10:B:22:G:N2       | 2.31                     | 0.46              |
| 18:E:54:MET:O       | 18:E:57:ILE:HG22   | 2.15                     | 0.46              |
| 19:F:67:ARG:HD3     | 19:F:67:ARG:N      | 2.31                     | 0.46              |
| 21:H:72:LEU:CD1     | 21:H:72:LEU:N      | 2.73                     | 0.46              |
| 40:a:1021:A:N3      | 40:a:1021:A:C3'    | 2.78                     | 0.46              |
| 40:a:2298:A:C6      | 40:a:2299:U:C2     | 3.04                     | 0.46              |
| 53:n:36:LEU:HB3     | 53:n:57:LEU:HD21   | 1.97                     | 0.46              |
| 8:7:12:G:H1'        | 14:AE:253:VAL:HG21 | 1.97                     | 0.46              |
| 9:9:43:LYS:HZ1      | 9:9:95:LEU:HD13    | 1.80                     | 0.46              |
| 10:A:14:A:H1'       | 10:A:22:G:N2       | 2.31                     | 0.46              |
| 10:A:18:G:O2'       | 10:A:60:U:N3       | 2.48                     | 0.46              |
| 10:A:41:C:C5'       | 26:M:143:ARG:HD2   | 2.46                     | 0.46              |
| 10:A:58:A:C1'       | 10:A:60:U:C5       | 2.99                     | 0.46              |
| 11:AA:103:VAL:HG12  | 11:AA:117:ILE:HG22 | 1.97                     | 0.46              |
| 11:AA:1314:GLN:HA   | 15:AF:28:ARG:HH22  | 1.80                     | 0.46              |
| 13:AD:35:PHE:HA     | 13:AD:38:THR:HG22  | 1.97                     | 0.46              |
| 14:AE:1341:ARG:NH1  | 14:AE:1343:GLU:OE2 | 2.49                     | 0.46              |
| 16:C:33:ILE:O       | 16:C:33:ILE:HG12   | 2.15                     | 0.46              |
| 9:9:139:LEU:HD21    | 39:Z:11:VAL:HG22   | 1.97                     | 0.46              |
| 14:AE:79:LYS:CB     | 14:AE:81:ARG:HH12  | 2.28                     | 0.46              |
| 14:AE:230:SER:OG    | 14:AE:231:GLY:N    | 2.49                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:G:16:PHE:CD2    | 21:H:42:LEU:O      | 2.69                     | 0.46              |
| 21:H:279:LYS:HA    | 21:H:331:MET:CB    | 2.33                     | 0.46              |
| 26:M:27:VAL:HG12   | 26:M:43:VAL:HG11   | 1.98                     | 0.46              |
| 28:O:63:LEU:HD13   | 28:O:65:ILE:HD11   | 1.97                     | 0.46              |
| 29:P:99:GLN:O      | 29:P:99:GLN:HG2    | 2.16                     | 0.46              |
| 40:a:1095:A:O2'    | 40:a:1096:A:O4'    | 2.33                     | 0.46              |
| 40:a:1720:U:H2'    | 40:a:1721:G:O4'    | 2.16                     | 0.46              |
| 40:a:1906:G:H4'    | 40:a:1906:G:OP1    | 2.16                     | 0.46              |
| 1:O:51:VAL:HG22    | 1:O:51:VAL:O       | 2.15                     | 0.46              |
| 12:AB:135:ARG:HG2  | 12:AB:135:ARG:HH11 | 1.80                     | 0.46              |
| 14:AE:516:ASP:OD1  | 14:AE:516:ASP:N    | 2.47                     | 0.46              |
| 14:AE:848:VAL:HB   | 14:AE:858:VAL:HG22 | 1.98                     | 0.46              |
| 14:AE:1321:SER:OG  | 14:AE:1349:GLU:OE2 | 2.32                     | 0.46              |
| 15:AF:25:ARG:NH1   | 15:AF:61:ASN:OD1   | 2.49                     | 0.46              |
| 17:D:1517:G:H1'    | 40:a:1919:A:O2'    | 2.16                     | 0.46              |
| 21:H:69:ASP:O      | 21:H:85:SER:CB     | 2.63                     | 0.46              |
| 40:a:2291:U:H2'    | 40:a:2292:U:C6     | 2.51                     | 0.46              |
| 9:9:43:LYS:NZ      | 9:9:95:LEU:HD13    | 2.30                     | 0.45              |
| 9:9:50:VAL:HG22    | 38:Y:119:ALA:C     | 2.41                     | 0.45              |
| 10:A:5:G:C2'       | 10:A:6:G:C5'       | 2.93                     | 0.45              |
| 12:AB:134:VAL:HG22 | 12:AB:160:VAL:HG11 | 1.98                     | 0.45              |
| 12:AB:147:VAL:HG23 | 12:AB:163:SER:HB3  | 1.92                     | 0.45              |
| 14:AE:59:ALA:HB3   | 14:AE:71:LEU:CD2   | 2.42                     | 0.45              |
| 10:B:18:G:O2'      | 10:B:60:U:N3       | 2.48                     | 0.45              |
| 17:D:868:C:H2'     | 17:D:869:G:O4'     | 2.16                     | 0.45              |
| 22:I:117:ALA:HB2   | 22:I:200:VAL:CG1   | 2.46                     | 0.45              |
| 35:V:8:LEU:HD23    | 35:V:25:ILE:HG21   | 1.97                     | 0.45              |
| 37:X:106:ALA:HB3   | 37:X:110:LYS:HD2   | 1.98                     | 0.45              |
| 38:Y:37:PHE:CE1    | 38:Y:56:VAL:HG11   | 2.51                     | 0.45              |
| 38:Y:79:LEU:HD13   | 38:Y:132:ALA:HA    | 1.97                     | 0.45              |
| 12:AB:144:PHE:HE2  | 29:P:81:GLU:CA     | 2.29                     | 0.45              |
| 12:AB:144:PHE:CD1  | 29:P:85:ASP:HB3    | 2.51                     | 0.45              |
| 12:AB:146:GLY:C    | 12:AB:163:SER:CB   | 2.76                     | 0.45              |
| 12:AB:148:VAL:O    | 12:AB:148:VAL:CG1  | 2.61                     | 0.45              |
| 17:D:1308:U:O5'    | 37:X:98:ARG:HG2    | 2.16                     | 0.45              |
| 38:Y:125:THR:HA    | 38:Y:128:ILE:HG12  | 1.98                     | 0.45              |
| 51:l:170:ARG:NH2   | 51:l:176:ASP:OD1   | 2.49                     | 0.45              |
| 58:s:30:THR:CG2    | 58:s:31:GLU:N      | 2.79                     | 0.45              |
| 8:7:14:U:H2'       | 8:7:15:G:C8        | 2.51                     | 0.45              |
| 10:A:60:U:OP2      | 10:A:61:C:N4       | 2.45                     | 0.45              |
| 11:AA:694:ARG:HH22 | 13:AC:80:GLU:HG3   | 1.82                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:AA:800:MET:HB2 | 11:AA:800:MET:HE3  | 1.69                     | 0.45              |
| 12:AB:133:MET:CG  | 12:AB:163:SER:CB   | 2.94                     | 0.45              |
| 14:AE:47:ARG:CG   | 29:P:81:GLU:OE1    | 2.64                     | 0.45              |
| 10:B:60:U:OP2     | 10:B:61:C:N4       | 2.45                     | 0.45              |
| 17:D:429:U:N3     | 17:D:431:A:N6      | 2.64                     | 0.45              |
| 20:G:114:LEU:HA   | 20:G:144:LEU:HD13  | 1.98                     | 0.45              |
| 37:X:16:VAL:HG23  | 37:X:17:ILE:HD12   | 1.97                     | 0.45              |
| 40:a:1363:C:O2'   | 40:a:1809:A:N3     | 2.46                     | 0.45              |
| 47:h:76:ALA:HB2   | 47:h:96:TYR:CD1    | 2.51                     | 0.45              |
| 7:6:15:DC:C4      | 7:6:16:DC:C5       | 3.05                     | 0.45              |
| 8:7:17:G:H2'      | 8:7:18:A:H8        | 1.80                     | 0.45              |
| 9:9:34:THR:HG22   | 9:9:38:MET:CE      | 2.46                     | 0.45              |
| 11:AA:712:SER:OG  | 11:AA:713:GLY:N    | 2.49                     | 0.45              |
| 13:AD:182:ARG:HD2 | 14:AE:581:MET:HE1  | 1.98                     | 0.45              |
| 17:D:1225:A:OP1   | 37:X:101:ARG:HB2   | 2.16                     | 0.45              |
| 17:D:1240:U:OP1   | 26:M:116:MET:HB2   | 2.16                     | 0.45              |
| 17:D:1397:C:O5'   | 17:D:1397:C:C6     | 2.70                     | 0.45              |
| 40:a:1007:C:OP1   | 58:s:37:ARG:NH2    | 2.50                     | 0.45              |
| 51:l:149:ILE:CD1  | 51:l:188:MET:HE3   | 2.46                     | 0.45              |
| 6:5:110:DA:N1     | 11:AA:536:GLY:O    | 2.50                     | 0.45              |
| 10:A:6:G:O2'      | 10:A:7:G:C5'       | 2.64                     | 0.45              |
| 12:AB:141:PHE:HD1 | 29:P:84:VAL:HG11   | 1.69                     | 0.45              |
| 13:AC:218:ARG:NH1 | 13:AD:231:PHE:O    | 2.50                     | 0.45              |
| 13:AD:185:TYR:HA  | 13:AD:202:VAL:O    | 2.16                     | 0.45              |
| 10:B:58:A:C1'     | 10:B:60:U:C5       | 2.99                     | 0.45              |
| 17:D:1340:A:H8    | 17:D:1340:A:O5'    | 1.99                     | 0.45              |
| 21:H:19:ARG:O     | 21:H:72:LEU:HD13   | 2.16                     | 0.45              |
| 21:H:135:LEU:CB   | 21:H:167:VAL:O     | 2.63                     | 0.45              |
| 45:f:25:LEU:C     | 45:f:25:LEU:HD13   | 2.41                     | 0.45              |
| 53:n:57:LEU:HD22  | 53:n:89:VAL:CG2    | 2.46                     | 0.45              |
| 10:A:19:G:C5      | 40:a:2112:G:H4'    | 2.44                     | 0.45              |
| 10:A:49:G:C2'     | 10:A:50:U:H5'      | 2.47                     | 0.45              |
| 11:AA:887:VAL:CG2 | 11:AA:913:VAL:HG21 | 2.46                     | 0.45              |
| 14:AE:41:PRO:HB2  | 14:AE:270:ARG:HG3  | 1.99                     | 0.45              |
| 40:a:2006:C:O2'   | 40:a:2823:A:N3     | 2.47                     | 0.45              |
| 40:a:2822:G:OP1   | 49:j:164:GLN:NE2   | 2.47                     | 0.45              |
| 43:d:48:U:H2'     | 43:d:49:C:C6       | 2.52                     | 0.45              |
| 49:j:186:LEU:HD21 | 64:y:4:ILE:HG21    | 1.98                     | 0.45              |
| 9:9:127:ALA:O     | 9:9:130:PRO:HG2    | 2.16                     | 0.45              |
| 10:A:48:C:N4      | 10:A:59:A:C5       | 2.84                     | 0.45              |
| 14:AE:68:TYR:CA   | 14:AE:92:VAL:HG23  | 2.45                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:D:526:C:OP2     | 31:R:88:LYS:HE3    | 2.15                     | 0.45              |
| 21:H:316:ILE:HD11  | 21:H:321:VAL:HG11  | 1.97                     | 0.45              |
| 37:X:75:MET:HA     | 37:X:75:MET:HE3    | 1.99                     | 0.45              |
| 37:X:106:ALA:HB3   | 37:X:110:LYS:CD    | 2.47                     | 0.45              |
| 39:Z:26:MET:HE2    | 39:Z:26:MET:HB2    | 1.71                     | 0.45              |
| 40:a:1067:A:O2'    | 40:a:1068:G:O4'    | 2.31                     | 0.45              |
| 40:a:2070:A:H2'    | 40:a:2071:A:O4'    | 2.16                     | 0.45              |
| 47:h:6:CYS:SG      | 47:h:13:ARG:NH1    | 2.89                     | 0.45              |
| 62:w:28:LEU:HD23   | 62:w:48:VAL:HG21   | 1.98                     | 0.45              |
| 10:A:76:A:C2       | 54:o:31:HIS:NE2    | 2.85                     | 0.45              |
| 11:AA:230:PHE:HB2  | 11:AA:333:ILE:HB   | 1.97                     | 0.45              |
| 12:AB:169:THR:CG2  | 29:P:84:VAL:HG13   | 2.43                     | 0.45              |
| 14:AE:482:ALA:HA   | 15:AF:6:VAL:HG21   | 1.98                     | 0.45              |
| 29:P:8:ILE:HD12    | 29:P:25:ILE:CD1    | 2.46                     | 0.45              |
| 40:a:995:C:O2      | 58:s:3:THR:OG1     | 2.24                     | 0.45              |
| 40:a:1394:U:H4'    | 40:a:1603:A:H4'    | 1.97                     | 0.45              |
| 57:r:55:GLU:HA     | 57:r:58:LEU:HD12   | 1.99                     | 0.45              |
| 8:7:14:U:H4'       | 14:AE:322:ARG:HH11 | 1.79                     | 0.45              |
| 9:9:50:VAL:CG2     | 38:Y:120:ASP:N     | 2.79                     | 0.45              |
| 9:9:106:PHE:CD2    | 9:9:106:PHE:O      | 2.70                     | 0.45              |
| 9:9:139:LEU:CD2    | 39:Z:11:VAL:HG22   | 2.47                     | 0.45              |
| 11:AA:735:LYS:HA   | 11:AA:748:ILE:HG22 | 1.98                     | 0.45              |
| 12:AB:173:LEU:HD13 | 12:AB:178:VAL:CG1  | 2.47                     | 0.45              |
| 13:AD:59:VAL:HG22  | 13:AD:144:ILE:HA   | 1.97                     | 0.45              |
| 14:AE:420:PRO:HA   | 14:AE:437:PHE:O    | 2.16                     | 0.45              |
| 10:B:34:C:C5       | 10:B:34:C:OP1      | 2.70                     | 0.45              |
| 17:D:337:G:H2'     | 17:D:338:A:C8      | 2.52                     | 0.45              |
| 20:G:114:LEU:HD13  | 20:G:144:LEU:CB    | 2.46                     | 0.45              |
| 21:H:294:VAL:HG21  | 21:H:330:VAL:HG21  | 1.99                     | 0.45              |
| 38:Y:95:ASP:OD2    | 38:Y:95:ASP:N      | 2.50                     | 0.45              |
| 38:Y:140:GLU:OE1   | 38:Y:140:GLU:N     | 2.50                     | 0.45              |
| 40:a:340:A:O2'     | 51:l:162:ARG:NH1   | 2.50                     | 0.45              |
| 40:a:1082:U:H3     | 40:a:1086:A:N6     | 2.15                     | 0.45              |
| 40:a:1327:A:H2'    | 40:a:1328:A:O4'    | 2.17                     | 0.45              |
| 40:a:1385:A:O2'    | 40:a:1396:U:O2     | 2.35                     | 0.45              |
| 53:n:29:PRO:HB2    | 53:n:169:LEU:HD22  | 1.99                     | 0.45              |
| 9:9:9:GLN:CD       | 9:9:9:GLN:C        | 2.85                     | 0.45              |
| 11:AA:674:ASP:OD2  | 11:AA:1070:HIS:ND1 | 2.50                     | 0.45              |
| 17:D:376:G:C2      | 17:D:389:A:C2      | 3.05                     | 0.45              |
| 21:H:290:TYR:O     | 21:H:305:HIS:C     | 2.56                     | 0.45              |
| 26:M:24:ALA:O      | 26:M:27:VAL:HG22   | 2.16                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:X:96:PRO:HG2   | 37:X:102:THR:HG23  | 1.97                     | 0.45              |
| 40:a:930:G:H1'    | 45:f:25:LEU:HD11   | 1.98                     | 0.45              |
| 63:x:18:LEU:HD23  | 63:x:25:ARG:HD2    | 1.99                     | 0.45              |
| 7:6:15:DC:N3      | 7:6:16:DC:C4       | 2.84                     | 0.44              |
| 8:7:-13:U:OP2     | 17:D:1397:C:O2     | 2.34                     | 0.44              |
| 9:9:106:PHE:O     | 9:9:106:PHE:CG     | 2.69                     | 0.44              |
| 11:AA:24:VAL:HG11 | 11:AA:704:MET:HE1  | 1.98                     | 0.44              |
| 10:B:37:A:N3      | 10:B:37:A:H5''     | 2.32                     | 0.44              |
| 10:B:48:C:C5      | 10:B:59:A:C8       | 3.05                     | 0.44              |
| 17:D:17:U:H2'     | 17:D:18:C:C6       | 2.52                     | 0.44              |
| 17:D:563:A:C2     | 17:D:884:U:O4      | 2.62                     | 0.44              |
| 17:D:1176:A:H2'   | 17:D:1177:G:O4'    | 2.16                     | 0.44              |
| 40:a:39:G:H1'     | 51:l:43:THR:HG21   | 1.99                     | 0.44              |
| 40:a:1927:A:C8    | 40:a:1927:A:O5'    | 2.71                     | 0.44              |
| 40:a:2898:U:O2'   | 58:s:134:ALA:O     | 2.28                     | 0.44              |
| 8:7:-12:U:C6      | 8:7:-12:U:OP2      | 2.70                     | 0.44              |
| 10:A:22:G:H2'     | 10:A:23:C:C5       | 2.52                     | 0.44              |
| 10:A:48:C:C5      | 10:A:59:A:C8       | 3.05                     | 0.44              |
| 13:AD:83:LEU:HD11 | 14:AE:526:VAL:HB   | 1.99                     | 0.44              |
| 10:B:25:C:C2'     | 10:B:26:G:H5'      | 2.47                     | 0.44              |
| 10:B:34:C:O5'     | 10:B:34:C:C6       | 2.70                     | 0.44              |
| 16:C:12:ARG:CZ    | 21:H:264:GLU:HA    | 2.46                     | 0.44              |
| 19:F:21:ARG:HH22  | 21:H:341:ARG:HD2   | 1.82                     | 0.44              |
| 21:H:33:LYS:HA    | 21:H:34:ASP:HA     | 1.61                     | 0.44              |
| 23:J:165:ARG:NH1  | 23:J:165:ARG:HB2   | 2.32                     | 0.44              |
| 38:Y:37:PHE:CD2   | 38:Y:37:PHE:O      | 2.70                     | 0.44              |
| 38:Y:42:ASN:HA    | 38:Y:45:THR:HB     | 1.98                     | 0.44              |
| 40:a:1589:U:C2    | 40:a:1590:A:C8     | 3.06                     | 0.44              |
| 57:r:15:LEU:HD13  | 57:r:15:LEU:C      | 2.42                     | 0.44              |
| 8:7:11:U:C4       | 8:7:11:U:OP2       | 2.70                     | 0.44              |
| 11:AA:557:ARG:HB3 | 11:AA:587:LEU:HD13 | 2.00                     | 0.44              |
| 11:AA:557:ARG:NH2 | 11:AA:607:SER:O    | 2.49                     | 0.44              |
| 11:AA:560:PRO:HB2 | 14:AE:776:THR:HG21 | 2.00                     | 0.44              |
| 13:AD:68:TYR:HE1  | 13:AD:79:LEU:HD13  | 1.82                     | 0.44              |
| 14:AE:774:ILE:HA  | 14:AE:777:HIS:HD2  | 1.82                     | 0.44              |
| 17:D:13:U:C2      | 17:D:915:A:C5      | 3.06                     | 0.44              |
| 17:D:915:A:H8     | 17:D:915:A:O5'     | 2.00                     | 0.44              |
| 17:D:1493:A:C8    | 17:D:1493:A:OP1    | 2.70                     | 0.44              |
| 18:E:55:GLN:N     | 18:E:56:PRO:HD2    | 2.32                     | 0.44              |
| 22:I:155:GLY:HA2  | 22:I:163:ALA:HB1   | 1.99                     | 0.44              |
| 38:Y:7:TYR:CD2    | 38:Y:7:TYR:O       | 2.70                     | 0.44              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 40:a:2638:G:O2'     | 40:a:2775:G:N2     | 2.41                     | 0.44              |
| 4:3:36:VAL:HG11     | 4:3:39:ILE:CD1     | 2.44                     | 0.44              |
| 7:6:21:DA:C6        | 8:7:15:G:C2        | 3.03                     | 0.44              |
| 9:9:111:ALA:HB3     | 9:9:114:GLU:HG3    | 1.98                     | 0.44              |
| 12:AB:64:PHE:HD2    | 12:AB:64:PHE:HA    | 1.67                     | 0.44              |
| 14:AE:388:ARG:NH2   | 14:AE:414:GLU:OE1  | 2.49                     | 0.44              |
| 10:B:57:A:O5'       | 10:B:58:A:P        | 2.76                     | 0.44              |
| 17:D:198:G:OP2      | 17:D:198:G:C8      | 2.70                     | 0.44              |
| 38:Y:124:MET:HE2    | 38:Y:124:MET:HB2   | 1.77                     | 0.44              |
| 40:a:954:G:OP2      | 61:v:16:ARG:NH2    | 2.50                     | 0.44              |
| 53:n:17:MET:HE2     | 53:n:25:VAL:HA     | 1.99                     | 0.44              |
| 65:z:76:TYR:OH      | 65:z:92:ARG:NH1    | 2.51                     | 0.44              |
| 9:9:106:PHE:CD2     | 9:9:106:PHE:C      | 2.95                     | 0.44              |
| 10:A:9:G:O2'        | 10:A:45:G:H2'      | 2.18                     | 0.44              |
| 10:A:56:C:OP1       | 40:a:2168:G:C4     | 2.71                     | 0.44              |
| 11:AA:641:GLU:OE2   | 14:AE:749:LYS:NZ   | 2.42                     | 0.44              |
| 12:AB:133:MET:SD    | 12:AB:145:ASN:CB   | 3.05                     | 0.44              |
| 10:B:49:G:C2'       | 10:B:50:U:H5'      | 2.47                     | 0.44              |
| 21:H:109:THR:C      | 21:H:153:GLU:HA    | 2.43                     | 0.44              |
| 23:J:197:GLU:HA     | 23:J:200:ILE:HD12  | 1.99                     | 0.44              |
| 11:AA:829:THR:HG23  | 11:AA:1059:ARG:HG2 | 1.99                     | 0.44              |
| 11:AA:1246:ARG:HH11 | 11:AA:1266:GLY:HA2 | 1.82                     | 0.44              |
| 10:B:9:G:O2'        | 10:B:45:G:H2'      | 2.18                     | 0.44              |
| 16:C:12:ARG:HD3     | 16:C:16:GLU:OE1    | 2.18                     | 0.44              |
| 17:D:109:A:C6       | 17:D:326:G:C6      | 3.05                     | 0.44              |
| 20:G:16:PHE:CG      | 21:H:43:LYS:HA     | 2.53                     | 0.44              |
| 37:X:23:TYR:CD2     | 37:X:69:LEU:HD23   | 2.53                     | 0.44              |
| 40:a:68:G:N2        | 40:a:74:A:OP2      | 2.49                     | 0.44              |
| 40:a:74:A:N7        | 40:a:88:G:C5       | 2.86                     | 0.44              |
| 2:1:17:VAL:HG12     | 2:1:76:VAL:HG21    | 1.98                     | 0.44              |
| 10:A:26:G:N2        | 10:A:45:G:N2       | 2.66                     | 0.44              |
| 11:AA:998:LEU:HG    | 11:AA:1011:LEU:HB3 | 1.99                     | 0.44              |
| 12:AB:65:PHE:HE2    | 12:AB:68:TYR:O     | 1.89                     | 0.44              |
| 17:D:324:G:N2       | 17:D:327:A:C8      | 2.86                     | 0.44              |
| 40:a:2547:A:H2'     | 40:a:2548:U:C6     | 2.52                     | 0.44              |
| 44:e:59:GLU:O       | 44:e:63:ALA:HB3    | 2.18                     | 0.44              |
| 6:5:116:DG:C6       | 6:5:117:DA:C6      | 3.06                     | 0.44              |
| 9:9:16:SER:HB2      | 9:9:20:LYS:NZ      | 2.33                     | 0.44              |
| 14:AE:975:ILE:HG22  | 14:AE:977:SER:H    | 1.83                     | 0.44              |
| 17:D:397:A:H3'      | 17:D:397:A:N3      | 2.33                     | 0.44              |
| 17:D:976:G:C8       | 17:D:1358:U:O2     | 2.71                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 20:G:206:ALA:O     | 20:G:210:VAL:HG23   | 2.18                     | 0.44              |
| 21:H:136:VAL:HA    | 21:H:168:VAL:O      | 2.18                     | 0.44              |
| 38:Y:121:ILE:HA    | 38:Y:124:MET:SD     | 2.58                     | 0.44              |
| 40:a:1386:C:H2'    | 40:a:1387:A:C8      | 2.53                     | 0.44              |
| 40:a:2395:C:H2'    | 40:a:2396:G:O4'     | 2.18                     | 0.44              |
| 7:6:12:DC:O5'      | 7:6:12:DC:H6        | 2.01                     | 0.44              |
| 9:9:72:LEU:HD22    | 9:9:72:LEU:C        | 2.42                     | 0.44              |
| 13:AD:29:GLU:HB3   | 13:AD:200:LYS:HG3   | 1.99                     | 0.44              |
| 14:AE:117:LEU:HG   | 14:AE:118:LYS:HG3   | 2.00                     | 0.44              |
| 17:D:842:U:H3'     | 17:D:843:U:C5'      | 2.48                     | 0.44              |
| 29:P:28:THR:HG21   | 29:P:87:LEU:HD12    | 1.99                     | 0.44              |
| 40:a:645:C:H2'     | 40:a:647:G:C8       | 2.52                     | 0.44              |
| 8:7:-9:U:C3'       | 8:7:-9:U:C6         | 3.00                     | 0.43              |
| 9:9:43:LYS:C       | 9:9:43:LYS:CD       | 2.86                     | 0.43              |
| 10:A:1:C:C5        | 10:A:2:G:N7         | 2.86                     | 0.43              |
| 14:AE:1036:ARG:HE  | 14:AE:1081:VAL:HG21 | 1.83                     | 0.43              |
| 10:B:22:G:H2'      | 10:B:23:C:C5        | 2.52                     | 0.43              |
| 10:B:26:G:N2       | 10:B:45:G:N2        | 2.66                     | 0.43              |
| 21:H:38:VAL:HG22   | 21:H:48:ILE:HD11    | 1.99                     | 0.43              |
| 38:Y:34:ILE:HG22   | 38:Y:34:ILE:O       | 2.18                     | 0.43              |
| 40:a:813:U:H2'     | 40:a:814:C:C6       | 2.53                     | 0.43              |
| 40:a:1925:C:C5     | 40:a:1925:C:OP2     | 2.70                     | 0.43              |
| 59:t:24:VAL:HG13   | 59:t:33:ALA:HB2     | 2.00                     | 0.43              |
| 9:9:52:MET:HE1     | 9:9:85:SER:HB2      | 2.00                     | 0.43              |
| 10:A:22:G:O2'      | 10:A:23:C:O5'       | 2.36                     | 0.43              |
| 10:A:57:A:O5'      | 10:A:58:A:P         | 2.76                     | 0.43              |
| 11:AA:300:ASP:OD1  | 11:AA:313:ALA:N     | 2.51                     | 0.43              |
| 11:AA:1157:GLN:HG3 | 11:AA:1159:VAL:HG13 | 2.00                     | 0.43              |
| 12:AB:136:VAL:HG11 | 12:AB:141:PHE:CB    | 2.48                     | 0.43              |
| 14:AE:438:GLU:OE2  | 14:AE:481:ARG:NH1   | 2.45                     | 0.43              |
| 14:AE:513:MET:HE2  | 14:AE:513:MET:HB3   | 1.79                     | 0.43              |
| 14:AE:907:HIS:ND1  | 14:AE:908:ILE:O     | 2.48                     | 0.43              |
| 20:G:35:ARG:CG     | 21:H:10:GLU:OE2     | 2.63                     | 0.43              |
| 40:a:2133:G:O2'    | 40:a:2157:G:N2      | 2.51                     | 0.43              |
| 46:g:37:CYS:N      | 46:g:40:CYS:SG      | 2.78                     | 0.43              |
| 9:9:71:CYS:CA      | 9:9:117:LEU:HD13    | 2.48                     | 0.43              |
| 14:AE:288:PRO:HG2  | 14:AE:291:ILE:HD12  | 2.00                     | 0.43              |
| 16:C:44:ILE:HG21   | 21:H:339:ARG:HA     | 2.01                     | 0.43              |
| 24:K:156:LYS:HG2   | 27:N:71:VAL:HG13    | 2.00                     | 0.43              |
| 40:a:1047:G:N2     | 40:a:1110:G:O2'     | 2.50                     | 0.43              |
| 40:a:2469:A:N6     | 40:a:2481:G:O2'     | 2.52                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 49:j:172:VAL:HG11   | 49:j:175:LEU:HD21   | 2.01                     | 0.43              |
| 8:7:11:U:OP2        | 8:7:11:U:C5         | 2.71                     | 0.43              |
| 10:A:34:C:OP1       | 26:M:84:THR:OG1     | 2.35                     | 0.43              |
| 11:AA:813:GLU:HB2   | 14:AE:461:PHE:HD2   | 1.83                     | 0.43              |
| 12:AB:148:VAL:HG22  | 12:AB:151:VAL:HG23  | 1.99                     | 0.43              |
| 10:B:22:G:O2'       | 10:B:23:C:O5'       | 2.36                     | 0.43              |
| 17:D:1515:G:H2'     | 17:D:1516:G:C8      | 2.52                     | 0.43              |
| 20:G:76:ALA:CB      | 20:G:210:VAL:HG11   | 2.47                     | 0.43              |
| 20:G:208:ARG:HH12   | 21:H:29:VAL:HG11    | 1.82                     | 0.43              |
| 24:K:153:VAL:HG23   | 24:K:164:ILE:HD13   | 2.00                     | 0.43              |
| 28:O:80:ARG:O       | 28:O:84:THR:HG23    | 2.17                     | 0.43              |
| 38:Y:116:MET:CB     | 38:Y:124:MET:HG2    | 2.46                     | 0.43              |
| 40:a:57:C:H2'       | 40:a:58:G:O4'       | 2.18                     | 0.43              |
| 40:a:998:C:OP2      | 65:z:58:ARG:NH2     | 2.49                     | 0.43              |
| 61:v:35:ALA:HB2     | 61:v:102:LEU:HD11   | 2.00                     | 0.43              |
| 10:A:58:A:HO2'      | 10:A:60:U:H5        | 1.63                     | 0.43              |
| 11:AA:11:ILE:HG22   | 11:AA:1172:LEU:HD11 | 2.00                     | 0.43              |
| 11:AA:811:ASN:ND2   | 11:AA:1098:LEU:O    | 2.51                     | 0.43              |
| 11:AA:1275:VAL:HG13 | 11:AA:1287:LEU:HD11 | 2.01                     | 0.43              |
| 11:AA:1313:HIS:CD2  | 15:AF:31:GLN:HE22   | 2.37                     | 0.43              |
| 13:AD:86:LYS:NZ     | 14:AE:532:GLU:OE2   | 2.41                     | 0.43              |
| 13:AD:192:VAL:HG12  | 13:AD:193:GLU:H     | 1.83                     | 0.43              |
| 10:B:18:G:N3        | 10:B:58:A:C5        | 2.87                     | 0.43              |
| 23:J:48:LEU:HD13    | 23:J:48:LEU:N       | 2.33                     | 0.43              |
| 40:a:1365:A:O5'     | 42:c:28:ARG:NH2     | 2.52                     | 0.43              |
| 4:3:12:ILE:CG2      | 4:3:80:ALA:HB2      | 2.49                     | 0.43              |
| 10:A:46:G:O2'       | 10:A:47:U:H5''      | 2.19                     | 0.43              |
| 12:AB:7:LYS:HG2     | 12:AB:74:VAL:HG13   | 2.01                     | 0.43              |
| 17:D:384:G:H2'      | 17:D:385:C:C6       | 2.54                     | 0.43              |
| 17:D:421:U:O2       | 17:D:421:U:O4'      | 2.37                     | 0.43              |
| 17:D:1499:A:O2'     | 17:D:1500:A:C5'     | 2.67                     | 0.43              |
| 20:G:114:LEU:HD13   | 20:G:144:LEU:HB3    | 1.99                     | 0.43              |
| 24:K:150:PRO:O      | 24:K:153:VAL:HG22   | 2.19                     | 0.43              |
| 47:h:37:ASN:HB2     | 47:h:62:TYR:HB2     | 2.01                     | 0.43              |
| 10:A:25:C:C2'       | 10:A:26:G:H5'       | 2.48                     | 0.43              |
| 11:AA:444:ASP:OD1   | 11:AA:444:ASP:N     | 2.51                     | 0.43              |
| 10:B:49:G:O5'       | 10:B:49:G:C8        | 2.71                     | 0.43              |
| 21:H:119:GLY:CA     | 21:H:132:PRO:C      | 2.92                     | 0.43              |
| 21:H:332:VAL:HG11   | 21:H:335:ILE:CG1    | 2.38                     | 0.43              |
| 62:w:49:GLU:HB2     | 62:w:50:PRO:HD3     | 2.01                     | 0.43              |
| 6:5:98:DA:C2'       | 6:5:99:DT:C7        | 2.96                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AA:678:ARG:HA   | 11:AA:678:ARG:HD3  | 1.84                     | 0.43              |
| 12:AB:128:PHE:HE1  | 12:AB:180:LYS:HD2  | 1.83                     | 0.43              |
| 12:AB:148:VAL:CG2  | 12:AB:151:VAL:CG2  | 2.96                     | 0.43              |
| 17:D:684:U:H2'     | 17:D:685:G:O4'     | 2.18                     | 0.43              |
| 21:H:335:ILE:HG12  | 21:H:342:ILE:HG23  | 2.00                     | 0.43              |
| 38:Y:64:ARG:HE     | 38:Y:64:ARG:HB2    | 1.52                     | 0.43              |
| 39:Z:18:ASP:HB3    | 39:Z:22:LEU:HD12   | 2.01                     | 0.43              |
| 40:a:1095:A:H2'    | 40:a:1096:A:C8     | 2.54                     | 0.43              |
| 10:A:18:G:N3       | 10:A:58:A:C5       | 2.87                     | 0.43              |
| 14:AE:47:ARG:CD    | 29:P:81:GLU:OE1    | 2.63                     | 0.43              |
| 10:B:46:G:O2'      | 10:B:47:U:H5''     | 2.19                     | 0.43              |
| 17:D:1371:G:O3'    | 28:O:71:GLY:HA3    | 2.19                     | 0.43              |
| 40:a:705:A:O4'     | 47:h:9:THR:HG21    | 2.19                     | 0.43              |
| 40:a:1142:A:N3     | 40:a:1142:A:H2'    | 2.34                     | 0.43              |
| 40:a:1921:G:C2'    | 40:a:1922:G:H5'    | 2.49                     | 0.43              |
| 52:m:12:ARG:HG3    | 52:m:44:VAL:HG11   | 2.00                     | 0.43              |
| 65:z:65:ILE:CD1    | 65:z:92:ARG:HB2    | 2.49                     | 0.43              |
| 12:AB:136:VAL:HG22 | 12:AB:178:VAL:HG12 | 2.01                     | 0.43              |
| 12:AB:141:PHE:CZ   | 29:P:84:VAL:HG21   | 2.53                     | 0.43              |
| 12:AB:142:ALA:O    | 12:AB:143:ASP:CB   | 2.63                     | 0.43              |
| 14:AE:658:GLU:HA   | 14:AE:661:VAL:HG22 | 2.00                     | 0.43              |
| 10:B:56:C:H2'      | 10:B:57:A:C5'      | 2.27                     | 0.43              |
| 16:C:12:ARG:O      | 16:C:16:GLU:HG3    | 2.19                     | 0.43              |
| 17:D:826:C:O2      | 27:N:16:ASN:ND2    | 2.52                     | 0.43              |
| 17:D:1333:A:H2'    | 17:D:1334:G:O4'    | 2.19                     | 0.43              |
| 40:a:126:A:O5'     | 52:m:19:ARG:HG3    | 2.19                     | 0.43              |
| 40:a:214:G:N2      | 40:a:216:A:N3      | 2.66                     | 0.43              |
| 40:a:1020:A:C2     | 40:a:1141:U:C2     | 3.07                     | 0.43              |
| 40:a:2252:G:O2'    | 40:a:2253:G:H5'    | 2.18                     | 0.43              |
| 58:s:32:LEU:HD23   | 58:s:54:ILE:HD13   | 2.01                     | 0.43              |
| 58:s:73:VAL:HG11   | 58:s:75:TYR:CZ     | 2.53                     | 0.43              |
| 59:t:113:MET:HE3   | 59:t:116:ILE:HD11  | 2.01                     | 0.43              |
| 3:2:1:MET:N        | 40:a:142:A:O2'     | 2.48                     | 0.42              |
| 8:7:-14:U:H6       | 8:7:-14:U:H3'      | 1.84                     | 0.42              |
| 11:AA:22:LEU:HB3   | 11:AA:655:VAL:HG11 | 2.01                     | 0.42              |
| 11:AA:1244:HIS:NE2 | 11:AA:1266:GLY:O   | 2.44                     | 0.42              |
| 15:AF:58:LEU:HD12  | 15:AF:59:ILE:HG12  | 2.00                     | 0.42              |
| 10:B:53:G:C2       | 10:B:54:U:C5       | 3.07                     | 0.42              |
| 10:B:58:A:OP2      | 10:B:58:A:H8       | 2.02                     | 0.42              |
| 17:D:1126:U:OP1    | 29:P:7:ARG:NH2     | 2.51                     | 0.42              |
| 17:D:1417:G:C6     | 17:D:1482:G:C6     | 3.06                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:H:302:GLY:HA3   | 21:H:344:LEU:HD13  | 2.00                     | 0.42              |
| 10:A:49:G:O5'      | 10:A:49:G:C8       | 2.71                     | 0.42              |
| 11:AA:125:GLY:H    | 11:AA:495:ALA:HB1  | 1.84                     | 0.42              |
| 12:AB:144:PHE:HB3  | 12:AB:162:VAL:CG1  | 2.49                     | 0.42              |
| 14:AE:47:ARG:NH2   | 29:P:81:GLU:CD     | 2.77                     | 0.42              |
| 14:AE:362:ARG:H    | 14:AE:365:GLN:HE21 | 1.66                     | 0.42              |
| 10:B:1:C:C5        | 10:B:2:G:N7        | 2.86                     | 0.42              |
| 17:D:37:U:O2       | 17:D:548:G:N2      | 2.53                     | 0.42              |
| 21:H:61:GLU:HG2    | 21:H:62:ILE:HG23   | 2.00                     | 0.42              |
| 29:P:57:VAL:O      | 29:P:58:ASN:ND2    | 2.53                     | 0.42              |
| 39:Z:29:LYS:HE2    | 39:Z:29:LYS:HB2    | 1.45                     | 0.42              |
| 40:a:1565:C:O2'    | 40:a:1567:G:N7     | 2.48                     | 0.42              |
| 59:t:38:ILE:HD11   | 59:t:112:PHE:CZ    | 2.54                     | 0.42              |
| 10:A:26:G:H1       | 10:A:44:A:N6       | 2.18                     | 0.42              |
| 11:AA:616:ILE:HG13 | 11:AA:652:TYR:HB2  | 2.02                     | 0.42              |
| 11:AA:646:SER:OG   | 11:AA:647:ARG:N    | 2.52                     | 0.42              |
| 11:AA:741:MET:HE3  | 11:AA:974:ARG:HH12 | 1.85                     | 0.42              |
| 14:AE:205:LEU:HD23 | 14:AE:205:LEU:HA   | 1.90                     | 0.42              |
| 14:AE:708:ASN:HA   | 14:AE:713:GLU:HA   | 2.00                     | 0.42              |
| 14:AE:859:PRO:HD2  | 14:AE:862:THR:HG21 | 2.01                     | 0.42              |
| 21:H:280:LEU:HB2   | 21:H:330:VAL:O     | 2.18                     | 0.42              |
| 38:Y:123:ALA:HA    | 38:Y:126:ARG:HG3   | 2.00                     | 0.42              |
| 40:a:2683:C:O2     | 59:t:70:ARG:NH2    | 2.52                     | 0.42              |
| 47:h:240:PHE:CD2   | 47:h:240:PHE:O     | 2.73                     | 0.42              |
| 60:u:109:LYS:HG2   | 60:u:126:ARG:HB2   | 2.01                     | 0.42              |
| 63:x:99:TYR:OH     | 63:x:111:ARG:NH1   | 2.53                     | 0.42              |
| 65:z:18:LEU:HD13   | 65:z:18:LEU:HA     | 1.95                     | 0.42              |
| 8:7:1:U:C3'        | 8:7:1:U:C6         | 3.02                     | 0.42              |
| 9:9:72:LEU:HD22    | 9:9:72:LEU:O       | 2.19                     | 0.42              |
| 12:AB:135:ARG:O    | 12:AB:178:VAL:CA   | 2.67                     | 0.42              |
| 12:AB:164:ILE:HD11 | 12:AB:168:ALA:CA   | 2.41                     | 0.42              |
| 14:AE:609:TYR:HD2  | 14:AE:610:ARG:HD2  | 1.85                     | 0.42              |
| 28:O:55:VAL:O      | 28:O:57:MET:N      | 2.52                     | 0.42              |
| 38:Y:41:PHE:HA     | 38:Y:68:PHE:CE2    | 2.54                     | 0.42              |
| 40:a:642:U:O2'     | 40:a:644:A:N7      | 2.51                     | 0.42              |
| 40:a:973:A:O4'     | 40:a:1188:U:C6     | 2.72                     | 0.42              |
| 53:n:123:ASP:OD1   | 53:n:123:ASP:C     | 2.62                     | 0.42              |
| 56:q:3:VAL:HA      | 56:q:36:ARG:O      | 2.19                     | 0.42              |
| 7:6:27:DG:H1'      | 7:6:28:DA:C5       | 2.55                     | 0.42              |
| 10:A:56:C:C2       | 40:a:2112:G:C5     | 3.07                     | 0.42              |
| 11:AA:478:ARG:HD2  | 11:AA:492:MET:HA   | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AD:31:LEU:HD21  | 13:AD:39:LEU:HD12  | 2.00                     | 0.42              |
| 13:AD:76:GLU:HB3   | 13:AD:80:GLU:HB3   | 2.01                     | 0.42              |
| 14:AE:211:GLU:HA   | 14:AE:214:ARG:HD2  | 2.01                     | 0.42              |
| 14:AE:694:SER:OG   | 14:AE:738:ARG:NE   | 2.52                     | 0.42              |
| 17:D:107:G:N7      | 18:E:10:ARG:NH2    | 2.60                     | 0.42              |
| 17:D:1323:G:H2'    | 17:D:1324:A:C8     | 2.54                     | 0.42              |
| 21:H:274:TYR:HD1   | 21:H:335:ILE:HD12  | 1.85                     | 0.42              |
| 22:I:50:ALA:HB2    | 22:I:75:ILE:HD12   | 2.00                     | 0.42              |
| 32:S:41:ARG:O      | 32:S:45:VAL:HG12   | 2.20                     | 0.42              |
| 38:Y:19:PRO:HG2    | 38:Y:24:GLY:N      | 2.32                     | 0.42              |
| 40:a:1932:A:H2'    | 40:a:1933:G:O4'    | 2.19                     | 0.42              |
| 40:a:2511:U:O4     | 40:a:2575:C:N3     | 2.52                     | 0.42              |
| 40:a:2615:U:C2     | 48:i:4:GLN:HA      | 2.55                     | 0.42              |
| 10:A:36:U:H2'      | 10:A:37:A:O4'      | 2.19                     | 0.42              |
| 10:A:53:G:C2       | 10:A:54:U:C5       | 3.07                     | 0.42              |
| 11:AA:590:PRO:HB2  | 11:AA:655:VAL:HG21 | 2.01                     | 0.42              |
| 14:AE:210:SER:O    | 14:AE:214:ARG:N    | 2.43                     | 0.42              |
| 14:AE:412:LEU:HA   | 14:AE:415:VAL:HG22 | 2.01                     | 0.42              |
| 14:AE:975:ILE:HD11 | 14:AE:1003:LEU:HG  | 2.02                     | 0.42              |
| 16:C:14:THR:CG2    | 16:C:48:ARG:HE     | 2.33                     | 0.42              |
| 21:H:119:GLY:O     | 21:H:120:PHE:C     | 2.62                     | 0.42              |
| 21:H:152:LEU:CB    | 21:H:171:ARG:H     | 2.32                     | 0.42              |
| 28:O:84:THR:HG21   | 28:O:103:PHE:CB    | 2.45                     | 0.42              |
| 33:T:21:ASP:OD1    | 33:T:22:THR:N      | 2.49                     | 0.42              |
| 40:a:1082:U:N3     | 40:a:1086:A:C6     | 2.87                     | 0.42              |
| 40:a:2803:G:H2'    | 40:a:2804:U:C5     | 2.55                     | 0.42              |
| 59:t:76:VAL:HG12   | 64:y:73:VAL:HB     | 2.00                     | 0.42              |
| 59:t:107:LEU:HD21  | 59:t:115:ILE:HG21  | 2.01                     | 0.42              |
| 13:AD:78:ILE:HA    | 13:AD:81:ILE:HG22  | 2.00                     | 0.42              |
| 14:AE:97:VAL:HG12  | 14:AE:101:ARG:HG3  | 2.02                     | 0.42              |
| 20:G:187:VAL:HG21  | 20:G:199:VAL:HG23  | 2.02                     | 0.42              |
| 21:H:76:GLU:HA     | 21:H:76:GLU:OE2    | 2.19                     | 0.42              |
| 30:Q:88:GLY:H      | 30:Q:114:THR:HG22  | 1.84                     | 0.42              |
| 40:a:67:U:C4       | 40:a:74:A:C6       | 3.04                     | 0.42              |
| 40:a:879:G:H2'     | 40:a:880:G:O4'     | 2.19                     | 0.42              |
| 40:a:2252:G:H2'    | 40:a:2253:G:H8     | 1.84                     | 0.42              |
| 46:g:18:CYS:HB2    | 46:g:40:CYS:HB3    | 1.96                     | 0.42              |
| 8:7:13:G:H5''      | 8:7:13:G:H8        | 1.85                     | 0.42              |
| 11:AA:524:ILE:HD12 | 11:AA:712:SER:HB2  | 2.02                     | 0.42              |
| 12:AB:136:VAL:HB   | 12:AB:141:PHE:O    | 2.20                     | 0.42              |
| 12:AB:175:PHE:O    | 12:AB:178:VAL:O    | 2.38                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 14:AE:79:LYS:HG3    | 14:AE:81:ARG:HH12   | 1.83                     | 0.42              |
| 14:AE:144:TYR:HH    | 14:AE:293:ARG:HH22  | 1.63                     | 0.42              |
| 14:AE:1155:ILE:HG13 | 14:AE:1210:ILE:HB   | 2.02                     | 0.42              |
| 17:D:429:U:O2       | 17:D:430:A:C8       | 2.72                     | 0.42              |
| 17:D:622:A:C8       | 17:D:623:C:C6       | 3.08                     | 0.42              |
| 21:H:19:ARG:CD      | 21:H:73:ASP:OD1     | 2.65                     | 0.42              |
| 40:a:631:A:N3       | 40:a:2415:G:O2'     | 2.48                     | 0.42              |
| 40:a:819:A:C4       | 40:a:1189:A:C2      | 3.07                     | 0.42              |
| 40:a:1925:C:OP2     | 40:a:1925:C:C6      | 2.73                     | 0.42              |
| 40:a:2602:A:H5''    | 40:a:2603:G:C5'     | 2.49                     | 0.42              |
| 51:l:48:THR:HG23    | 51:l:86:ALA:HB3     | 2.02                     | 0.42              |
| 51:l:145:ASP:HA     | 51:l:166:LYS:HB3    | 2.02                     | 0.42              |
| 8:7:-20:A:H2'       | 8:7:-19:U:C6        | 2.50                     | 0.42              |
| 9:9:18:VAL:HA       | 9:9:86:MET:CE       | 2.44                     | 0.42              |
| 9:9:25:ALA:HA       | 9:9:96:PHE:HE1      | 1.85                     | 0.42              |
| 14:AE:641:ILE:HD12  | 14:AE:641:ILE:HA    | 1.89                     | 0.42              |
| 17:D:972:C:O2'      | 29:P:57:VAL:HG21    | 2.18                     | 0.42              |
| 24:K:136:VAL:O      | 24:K:140:THR:HG23   | 2.20                     | 0.42              |
| 26:M:22:LEU:HD13    | 26:M:97:ASN:ND2     | 2.35                     | 0.42              |
| 28:O:28:ILE:HD12    | 28:O:28:ILE:N       | 2.35                     | 0.42              |
| 34:U:6:LEU:HG       | 34:U:17:TYR:HB3     | 2.00                     | 0.42              |
| 40:a:126:A:OP1      | 52:m:45:SER:OG      | 2.38                     | 0.42              |
| 48:i:43:ILE:HG22    | 48:i:49:TYR:HB2     | 2.01                     | 0.42              |
| 8:7:-8:U:C6         | 8:7:-8:U:C3'        | 3.03                     | 0.42              |
| 11:AA:699:LEU:HG    | 11:AA:799:ASN:HD22  | 1.85                     | 0.42              |
| 12:AB:103:ILE:HG13  | 12:AB:104:SER:H     | 1.85                     | 0.42              |
| 14:AE:1272:SER:HB2  | 14:AE:1292:LEU:HD11 | 2.02                     | 0.42              |
| 17:D:977:A:H1'      | 17:D:982:U:O4       | 2.20                     | 0.42              |
| 17:D:1208:C:H2'     | 17:D:1209:C:H6      | 1.85                     | 0.42              |
| 17:D:1329:A:OP1     | 37:X:28:THR:CA      | 2.67                     | 0.42              |
| 40:a:1028:A:N6      | 40:a:1125:G:H2'     | 2.34                     | 0.42              |
| 40:a:1394:U:C4      | 40:a:1395:A:C6      | 3.07                     | 0.42              |
| 40:a:1570:A:H2'     | 40:a:1571:A:C8      | 2.55                     | 0.42              |
| 40:a:2311:A:C2      | 53:n:85:ILE:HD11    | 2.55                     | 0.42              |
| 40:a:2756:U:C4      | 40:a:2759:G:O6      | 2.72                     | 0.42              |
| 40:a:2788:C:H2'     | 40:a:2789:C:C6      | 2.55                     | 0.42              |
| 42:c:37:ARG:HG2     | 42:c:48:THR:HG23    | 2.00                     | 0.42              |
| 4:3:39:ILE:HG22     | 4:3:40:ASN:N        | 2.34                     | 0.41              |
| 9:9:80:THR:O        | 40:a:1108:U:OP1     | 2.38                     | 0.41              |
| 14:AE:66:LYS:HB2    | 14:AE:69:GLU:HB2    | 2.02                     | 0.41              |
| 14:AE:79:LYS:CB     | 14:AE:81:ARG:NH1    | 2.73                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:D:548:G:C6      | 17:D:549:C:C4      | 3.08                     | 0.41              |
| 19:F:32:VAL:HG11   | 30:Q:89:PRO:HG3    | 2.01                     | 0.41              |
| 38:Y:10:LEU:HD13   | 38:Y:10:LEU:HA     | 1.79                     | 0.41              |
| 40:a:320:A:H2'     | 51:l:131:THR:HG21  | 2.01                     | 0.41              |
| 40:a:948:C:H1'     | 40:a:984:A:C8      | 2.55                     | 0.41              |
| 3:2:46:ALA:O       | 3:2:50:LEU:HB2     | 2.20                     | 0.41              |
| 10:A:56:C:H2'      | 10:A:57:A:C5'      | 2.27                     | 0.41              |
| 14:AE:289:ASP:HA   | 14:AE:292:VAL:HG22 | 2.01                     | 0.41              |
| 14:AE:708:ASN:N    | 14:AE:708:ASN:OD1  | 2.50                     | 0.41              |
| 17:D:502:A:H2'     | 17:D:503:C:O4'     | 2.20                     | 0.41              |
| 21:H:155:LYS:O     | 21:H:169:SER:CB    | 2.69                     | 0.41              |
| 38:Y:102:ARG:H     | 38:Y:102:ARG:HG3   | 1.59                     | 0.41              |
| 40:a:36:G:N3       | 40:a:450:G:O2'     | 2.53                     | 0.41              |
| 40:a:783:A:N3      | 40:a:783:A:C2'     | 2.70                     | 0.41              |
| 47:h:76:ALA:HB2    | 47:h:96:TYR:CE1    | 2.55                     | 0.41              |
| 51:l:134:LEU:HB2   | 51:l:160:ALA:HB1   | 2.02                     | 0.41              |
| 52:m:12:ARG:CG     | 52:m:44:VAL:HG11   | 2.50                     | 0.41              |
| 8:7:13:G:H8        | 8:7:13:G:C5'       | 2.33                     | 0.41              |
| 9:9:31:ARG:HD3     | 9:9:31:ARG:HA      | 1.92                     | 0.41              |
| 9:9:61:ARG:C       | 9:9:65:GLU:HB2     | 2.45                     | 0.41              |
| 11:AA:27:LEU:O     | 11:AA:528:ARG:NH1  | 2.43                     | 0.41              |
| 11:AA:144:VAL:HG23 | 11:AA:515:MET:HB2  | 2.02                     | 0.41              |
| 11:AA:469:VAL:HA   | 11:AA:472:GLU:HG2  | 2.01                     | 0.41              |
| 12:AB:144:PHE:HZ   | 29:P:81:GLU:O      | 1.97                     | 0.41              |
| 13:AD:46:ILE:HD11  | 13:AD:224:LEU:HD13 | 2.02                     | 0.41              |
| 10:B:65:C:C2'      | 10:B:66:C:H5'      | 2.49                     | 0.41              |
| 17:D:662:U:O2'     | 17:D:836:G:OP1     | 2.32                     | 0.41              |
| 17:D:860:A:H2'     | 17:D:861:G:O4'     | 2.20                     | 0.41              |
| 17:D:915:A:C6      | 17:D:916:U:C4      | 3.08                     | 0.41              |
| 20:G:208:ARG:NH1   | 21:H:29:VAL:HG11   | 2.34                     | 0.41              |
| 33:T:43:PHE:CE2    | 33:T:56:LEU:HD22   | 2.55                     | 0.41              |
| 39:Z:1:SER:HB3     | 39:Z:2:ILE:H       | 1.61                     | 0.41              |
| 40:a:1250:G:OP2    | 60:u:21:ARG:NH2    | 2.53                     | 0.41              |
| 40:a:2273:A:H2'    | 40:a:2274:A:C8     | 2.55                     | 0.41              |
| 9:9:8:LYS:HZ1      | 40:a:1046:A:H61    | 1.68                     | 0.41              |
| 10:A:56:C:OP1      | 40:a:2168:G:N3     | 2.53                     | 0.41              |
| 10:A:58:A:OP2      | 10:A:58:A:H8       | 2.02                     | 0.41              |
| 11:AA:746:ALA:O    | 11:AA:974:ARG:NH2  | 2.45                     | 0.41              |
| 17:D:429:U:O2      | 17:D:430:A:N7      | 2.53                     | 0.41              |
| 20:G:19:GLN:HG2    | 21:H:75:VAL:HG22   | 1.91                     | 0.41              |
| 20:G:47:VAL:N      | 20:G:48:PRO:HD2    | 2.34                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 24:K:133:PRO:HA    | 24:K:136:VAL:HG12   | 2.02                     | 0.41              |
| 40:a:476:G:H4'     | 40:a:502:A:N1       | 2.35                     | 0.41              |
| 40:a:567:U:OP2     | 60:u:29:LYS:NZ      | 2.53                     | 0.41              |
| 40:a:984:A:N3      | 40:a:984:A:H2'      | 2.35                     | 0.41              |
| 40:a:1169:A:H5''   | 40:a:1169:A:N3      | 2.36                     | 0.41              |
| 40:a:1182:G:H2'    | 40:a:1183:U:O4'     | 2.21                     | 0.41              |
| 40:a:1548:A:H2'    | 40:a:1549:A:C8      | 2.55                     | 0.41              |
| 40:a:2294:G:OP1    | 63:x:10:ARG:HD3     | 2.21                     | 0.41              |
| 53:n:122:PHE:CZ    | 53:n:167:ARG:HA     | 2.56                     | 0.41              |
| 9:9:48:ALA:HB3     | 9:9:51:TYR:HD2      | 1.86                     | 0.41              |
| 11:AA:310:ILE:HG21 | 11:AA:325:LEU:HB3   | 2.03                     | 0.41              |
| 10:B:26:G:H1       | 10:B:44:A:N6        | 2.18                     | 0.41              |
| 10:B:47:U:O2'      | 10:B:50:U:OP1       | 2.37                     | 0.41              |
| 17:D:1225:A:H2'    | 17:D:1226:C:C5      | 2.56                     | 0.41              |
| 21:H:342:ILE:HG22  | 21:H:344:LEU:HD12   | 2.01                     | 0.41              |
| 31:R:110:ARG:NH1   | 31:R:112:GLN:O      | 2.53                     | 0.41              |
| 38:Y:102:ARG:HD2   | 38:Y:103:ALA:N      | 2.36                     | 0.41              |
| 40:a:1406:U:C2'    | 40:a:1407:G:OP2     | 2.69                     | 0.41              |
| 40:a:2602:A:H5''   | 40:a:2603:G:H5''    | 2.03                     | 0.41              |
| 65:z:66:ASN:OD1    | 65:z:70:ARG:NE      | 2.54                     | 0.41              |
| 9:9:72:LEU:C       | 9:9:72:LEU:CD2      | 2.94                     | 0.41              |
| 13:AD:205:MET:HE1  | 13:AD:217:ILE:HG13  | 2.03                     | 0.41              |
| 10:B:46:G:H2'      | 10:B:47:U:OP2       | 2.21                     | 0.41              |
| 17:D:1330:U:OP2    | 37:X:26:GLY:HA3     | 2.21                     | 0.41              |
| 22:I:9:GLY:HA3     | 32:S:89:MET:HE3     | 2.02                     | 0.41              |
| 27:N:11:LEU:HD22   | 27:N:75:ILE:HD11    | 2.03                     | 0.41              |
| 37:X:4:ILE:CG1     | 37:X:9:ILE:HD12     | 2.50                     | 0.41              |
| 40:a:17:G:H2'      | 40:a:18:U:C6        | 2.56                     | 0.41              |
| 58:s:114:LEU:HD12  | 58:s:114:LEU:HA     | 1.87                     | 0.41              |
| 62:w:29:VAL:HG11   | 62:w:75:ILE:HG23    | 2.03                     | 0.41              |
| 9:9:3:LEU:N        | 9:9:3:LEU:CD1       | 2.73                     | 0.41              |
| 10:A:7:G:O6        | 10:A:49:G:O6        | 2.39                     | 0.41              |
| 10:A:26:G:C2       | 10:A:45:G:N2        | 2.89                     | 0.41              |
| 11:AA:135:THR:HG22 | 11:AA:144:VAL:HG22  | 2.03                     | 0.41              |
| 11:AA:741:MET:SD   | 11:AA:974:ARG:NH2   | 2.93                     | 0.41              |
| 11:AA:861:ALA:HB1  | 11:AA:882:ILE:HD13  | 2.01                     | 0.41              |
| 11:AA:936:ARG:HB2  | 11:AA:1042:LEU:HD12 | 2.03                     | 0.41              |
| 14:AE:513:MET:HE1  | 14:AE:579:LEU:HD13  | 2.01                     | 0.41              |
| 14:AE:789:LYS:HB2  | 14:AE:789:LYS:HE2   | 1.89                     | 0.41              |
| 10:B:15:G:N2       | 10:B:20:U:C2        | 2.88                     | 0.41              |
| 23:J:100:ASN:OD1   | 23:J:111:ARG:NH1    | 2.54                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:a:493:G:H2'     | 40:a:494:G:O4'     | 2.20                     | 0.41              |
| 40:a:548:G:H3'     | 40:a:549:G:O4'     | 2.20                     | 0.41              |
| 40:a:2189:U:O2'    | 40:a:2190:G:O4'    | 2.36                     | 0.41              |
| 40:a:2298:A:C5     | 40:a:2321:U:C4     | 3.09                     | 0.41              |
| 47:h:119:GLY:O     | 47:h:130:LEU:HB3   | 2.20                     | 0.41              |
| 12:AB:146:GLY:CA   | 12:AB:163:SER:HB2  | 2.36                     | 0.41              |
| 14:AE:1022:PRO:O   | 14:AE:1126:GLN:NE2 | 2.45                     | 0.41              |
| 38:Y:23:VAL:HB     | 38:Y:24:GLY:H      | 1.65                     | 0.41              |
| 40:a:1839:G:C4     | 40:a:1927:A:C5     | 3.08                     | 0.41              |
| 62:w:67:PHE:O      | 62:w:71:ARG:HG2    | 2.21                     | 0.41              |
| 2:1:75:PHE:CZ      | 2:1:104:THR:HG21   | 2.56                     | 0.41              |
| 9:9:73:LYS:CB      | 9:9:117:LEU:HD11   | 2.51                     | 0.41              |
| 9:9:118:ILE:H      | 9:9:119:PRO:HD2    | 1.85                     | 0.41              |
| 10:A:15:G:H1       | 10:A:20:U:H3       | 1.68                     | 0.41              |
| 10:A:34:C:H41      | 26:M:83:SER:HA     | 1.86                     | 0.41              |
| 10:A:46:G:O2'      | 10:A:47:U:C6       | 2.73                     | 0.41              |
| 11:AA:998:LEU:HD21 | 11:AA:1015:ALA:HB2 | 2.02                     | 0.41              |
| 12:AB:64:PHE:CZ    | 14:AE:285:LEU:CD2  | 3.04                     | 0.41              |
| 14:AE:138:VAL:HG21 | 14:AE:145:VAL:HB   | 2.03                     | 0.41              |
| 10:B:7:G:O6        | 10:B:49:G:O6       | 2.39                     | 0.41              |
| 10:B:8:U:H6        | 10:B:8:U:OP2       | 2.04                     | 0.41              |
| 10:B:26:G:C2       | 10:B:45:G:N2       | 2.88                     | 0.41              |
| 16:C:12:ARG:HH22   | 21:H:268:VAL:HG21  | 1.82                     | 0.41              |
| 17:D:152:A:N6      | 17:D:170:U:C2      | 2.89                     | 0.41              |
| 17:D:580:C:H2'     | 17:D:581:G:O4'     | 2.21                     | 0.41              |
| 17:D:791:G:N2      | 17:D:1497:G:O3'    | 2.53                     | 0.41              |
| 17:D:1061:G:H5'    | 29:P:61:ALA:HB2    | 2.02                     | 0.41              |
| 21:H:292:CYS:SG    | 21:H:304:VAL:HB    | 2.60                     | 0.41              |
| 37:X:16:VAL:HG13   | 37:X:34:LEU:CD1    | 2.51                     | 0.41              |
| 40:a:5:A:H2'       | 40:a:6:A:C8        | 2.56                     | 0.41              |
| 40:a:851:C:H2'     | 40:a:852:U:C6      | 2.55                     | 0.41              |
| 40:a:1082:U:C4     | 40:a:1086:A:N6     | 2.88                     | 0.41              |
| 40:a:2641:G:OP1    | 58:s:78:THR:HG22   | 2.21                     | 0.41              |
| 49:j:175:LEU:CD1   | 49:j:193:VAL:HG12  | 2.51                     | 0.41              |
| 55:p:52:PHE:CZ     | 55:p:72:LEU:HD22   | 2.56                     | 0.41              |
| 61:v:73:ILE:HG21   | 61:v:91:TYR:CZ     | 2.55                     | 0.41              |
| 8:7:-11:U:O2       | 8:7:-11:U:C3'      | 2.69                     | 0.41              |
| 9:9:71:CYS:SG      | 9:9:117:LEU:HB2    | 2.60                     | 0.41              |
| 11:AA:374:GLU:HB2  | 12:AB:80:TRP:CH2   | 2.56                     | 0.41              |
| 14:AE:134:ASP:HB3  | 14:AE:159:ILE:HG21 | 2.02                     | 0.41              |
| 17:D:197:A:C5      | 17:D:221:C:H4'     | 2.53                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 17:D:216:U:H2'      | 17:D:217:C:C6      | 2.55                     | 0.41              |
| 17:D:218:U:H2'      | 17:D:219:U:O4'     | 2.21                     | 0.41              |
| 17:D:915:A:C8       | 17:D:915:A:C3'     | 3.04                     | 0.41              |
| 17:D:1370:G:C2      | 17:D:1371:G:C8     | 3.09                     | 0.41              |
| 21:H:110:GLY:H      | 21:H:153:GLU:N     | 2.17                     | 0.41              |
| 38:Y:133:ARG:HG3    | 38:Y:136:GLY:HA2   | 2.03                     | 0.41              |
| 40:a:871:U:H2'      | 40:a:872:U:C6      | 2.56                     | 0.41              |
| 40:a:1736:U:H2'     | 40:a:1737:G:O4'    | 2.21                     | 0.41              |
| 8:7:-7:U:OP1        | 22:I:129:MET:HE1   | 2.21                     | 0.40              |
| 9:9:8:LYS:NZ        | 40:a:1046:A:N6     | 2.69                     | 0.40              |
| 10:A:8:U:OP2        | 10:A:8:U:H6        | 2.04                     | 0.40              |
| 13:AC:42:ALA:HB1    | 13:AC:224:LEU:HD11 | 2.03                     | 0.40              |
| 13:AC:104:LYS:HG2   | 13:AC:110:VAL:HG22 | 2.03                     | 0.40              |
| 14:AE:246:PRO:HA    | 14:AE:247:PRO:HD3  | 1.93                     | 0.40              |
| 14:AE:800:LEU:HB3   | 14:AE:920:ALA:HB1  | 2.02                     | 0.40              |
| 14:AE:847:ASP:OD1   | 14:AE:847:ASP:N    | 2.54                     | 0.40              |
| 10:B:37:A:H5''      | 10:B:37:A:C4       | 2.56                     | 0.40              |
| 17:D:1368:A:OP1     | 28:O:113:ARG:NH2   | 2.54                     | 0.40              |
| 19:F:67:ARG:HD3     | 19:F:67:ARG:H      | 1.85                     | 0.40              |
| 25:L:27:ALA:O       | 25:L:30:THR:OG1    | 2.32                     | 0.40              |
| 40:a:197:A:N6       | 40:a:2430:A:H2'    | 2.36                     | 0.40              |
| 43:d:39:A:O2'       | 43:d:46:A:N1       | 2.49                     | 0.40              |
| 51:l:149:ILE:HD11   | 51:l:188:MET:HE3   | 2.02                     | 0.40              |
| 55:p:25:THR:HG22    | 55:p:34:THR:HG23   | 2.02                     | 0.40              |
| 10:A:25:C:H2'       | 10:A:26:G:C5'      | 2.51                     | 0.40              |
| 10:A:46:G:H2'       | 10:A:47:U:OP2      | 2.21                     | 0.40              |
| 11:AA:845:LEU:HD12  | 11:AA:909:LYS:NZ   | 2.37                     | 0.40              |
| 13:AC:57:THR:HG23   | 13:AC:158:ARG:HH21 | 1.86                     | 0.40              |
| 14:AE:47:ARG:HH21   | 29:P:81:GLU:HB3    | 1.87                     | 0.40              |
| 14:AE:79:LYS:HB3    | 14:AE:79:LYS:NZ    | 2.36                     | 0.40              |
| 14:AE:836:ARG:HG3   | 14:AE:869:CYS:HB3  | 2.02                     | 0.40              |
| 14:AE:964:LYS:O     | 14:AE:976:THR:OG1  | 2.35                     | 0.40              |
| 14:AE:1003:LEU:HD23 | 14:AE:1018:ALA:HB2 | 2.02                     | 0.40              |
| 17:D:1526:G:P       | 19:F:42:THR:HG23   | 2.61                     | 0.40              |
| 21:H:123:GLU:CA     | 21:H:128:ARG:HA    | 2.43                     | 0.40              |
| 21:H:286:ASN:OD1    | 21:H:286:ASN:N     | 2.55                     | 0.40              |
| 21:H:332:VAL:HG12   | 21:H:334:ASP:N     | 2.33                     | 0.40              |
| 24:K:150:PRO:HA     | 24:K:153:VAL:HG22  | 2.03                     | 0.40              |
| 38:Y:35:MET:O       | 38:Y:35:MET:SD     | 2.79                     | 0.40              |
| 38:Y:52:LEU:HD21    | 38:Y:81:LYS:HD3    | 2.03                     | 0.40              |
| 40:a:829:A:N7       | 40:a:2247:A:O2'    | 2.49                     | 0.40              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 40:a:1421:G:C2     | 40:a:1422:G:C8      | 3.09                     | 0.40              |
| 9:9:23:LEU:HA      | 9:9:118:ILE:CG1     | 2.51                     | 0.40              |
| 11:AA:1069:ARG:NH2 | 11:AA:1114:GLU:OE2  | 2.44                     | 0.40              |
| 14:AE:319:SER:HA   | 14:AE:320:ASN:HA    | 1.74                     | 0.40              |
| 14:AE:367:GLY:HA3  | 14:AE:448:GLN:HB2   | 2.03                     | 0.40              |
| 14:AE:591:ILE:HG23 | 14:AE:592:VAL:HG13  | 2.03                     | 0.40              |
| 17:D:1235:U:H2'    | 17:D:1236:A:O4'     | 2.20                     | 0.40              |
| 36:W:50:ALA:HB1    | 36:W:57:HIS:HB3     | 2.04                     | 0.40              |
| 37:X:16:VAL:O      | 37:X:20:THR:HG23    | 2.21                     | 0.40              |
| 38:Y:24:GLY:HA3    | 38:Y:25:PRO:HD3     | 1.93                     | 0.40              |
| 40:a:742:A:N1      | 40:a:755:U:O4       | 2.53                     | 0.40              |
| 2:1:92:ARG:NE      | 2:1:94:ASP:OD1      | 2.53                     | 0.40              |
| 8:7:11:U:O2        | 11:AA:1253:LEU:CD1  | 2.38                     | 0.40              |
| 9:9:47:GLU:HG3     | 9:9:95:LEU:CD2      | 2.49                     | 0.40              |
| 11:AA:836:LEU:HD21 | 11:AA:921:PRO:HD3   | 2.02                     | 0.40              |
| 11:AA:979:LEU:HD11 | 11:AA:1011:LEU:HD11 | 2.03                     | 0.40              |
| 11:AA:1105:SER:HB2 | 14:AE:731:ARG:HB3   | 2.03                     | 0.40              |
| 12:AB:127:LEU:CD1  | 12:AB:153:TYR:OH    | 2.67                     | 0.40              |
| 12:AB:135:ARG:O    | 12:AB:179:GLU:N     | 2.53                     | 0.40              |
| 12:AB:157:ARG:HD2  | 12:AB:172:GLU:HB3   | 2.02                     | 0.40              |
| 12:AB:170:PRO:CD   | 29:P:100:ILE:HB     | 2.17                     | 0.40              |
| 10:B:15:G:H1       | 10:B:20:U:H3        | 1.68                     | 0.40              |
| 10:B:25:C:H2'      | 10:B:26:G:C5'       | 2.51                     | 0.40              |
| 10:B:76:A:N3       | 40:a:2493:U:H5''    | 2.37                     | 0.40              |
| 17:D:236:A:H5''    | 35:V:44:LEU:HD21    | 2.04                     | 0.40              |
| 17:D:579:A:O2'     | 33:T:54:ARG:NH1     | 2.54                     | 0.40              |
| 24:K:154:ALA:HA    | 24:K:164:ILE:HD11   | 2.03                     | 0.40              |
| 57:r:9:VAL:HG11    | 57:r:12:LEU:HD21    | 2.03                     | 0.40              |
| 8:7:-20:A:C6       | 8:7:-19:U:C4        | 3.09                     | 0.40              |
| 10:A:15:G:N2       | 10:A:20:U:H3        | 2.20                     | 0.40              |
| 11:AA:159:SER:HB2  | 11:AA:442:VAL:HG11  | 2.04                     | 0.40              |
| 12:AB:141:PHE:CE1  | 12:AB:169:THR:HG21  | 2.52                     | 0.40              |
| 13:AD:205:MET:HE2  | 13:AD:205:MET:HB3   | 1.89                     | 0.40              |
| 14:AE:706:VAL:HG12 | 14:AE:715:LYS:HB3   | 2.04                     | 0.40              |
| 17:D:1255:G:O2'    | 17:D:1258:G:N3      | 2.47                     | 0.40              |
| 21:H:70:VAL:CA     | 21:H:85:SER:HA      | 2.50                     | 0.40              |
| 26:M:27:VAL:HG12   | 26:M:43:VAL:HG21    | 2.04                     | 0.40              |
| 28:O:10:GLY:HA3    | 28:O:78:ALA:O       | 2.21                     | 0.40              |
| 29:P:87:LEU:HD12   | 29:P:87:LEU:HA      | 1.87                     | 0.40              |
| 38:Y:14:ALA:HB3    | 38:Y:50:LYS:HA      | 2.03                     | 0.40              |
| 40:a:753:A:C5      | 40:a:754:U:C5       | 3.09                     | 0.40              |

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| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 40:a:2315:G:C5' | 53:n:157:THR:HG23 | 2.52                     | 0.40              |
| 53:n:4:LEU:HD23 | 53:n:4:LEU:HA     | 1.96                     | 0.40              |
| 57:r:57:LYS:O   | 57:r:61:VAL:HG13  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 1   | 0     | 101/103 (98%)    | 97 (96%)   | 3 (3%)   | 1 (1%)   | 12          | 47  |
| 2   | 1     | 108/110 (98%)    | 104 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 3   | 2     | 92/100 (92%)     | 90 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 4   | 3     | 101/104 (97%)    | 96 (95%)   | 4 (4%)   | 1 (1%)   | 12          | 47  |
| 5   | 4     | 92/94 (98%)      | 91 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 9   | 9     | 146/165 (88%)    | 95 (65%)   | 37 (25%) | 14 (10%) | 0           | 7   |
| 11  | AA    | 1338/1342 (100%) | 1219 (91%) | 115 (9%) | 4 (0%)   | 36          | 72  |
| 12  | AB    | 173/181 (96%)    | 138 (80%)  | 26 (15%) | 9 (5%)   | 1           | 14  |
| 13  | AC    | 217/329 (66%)    | 203 (94%)  | 12 (6%)  | 2 (1%)   | 14          | 50  |
| 13  | AD    | 214/329 (65%)    | 198 (92%)  | 16 (8%)  | 0        | 100         | 100 |
| 14  | AE    | 1331/1407 (95%)  | 1218 (92%) | 110 (8%) | 3 (0%)   | 43          | 77  |
| 15  | AF    | 80/91 (88%)      | 77 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 16  | C     | 64/75 (85%)      | 63 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 18  | E     | 84/87 (97%)      | 83 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 19  | F     | 68/71 (96%)      | 68 (100%)  | 0        | 0        | 100         | 100 |
| 20  | G     | 223/241 (92%)    | 210 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 21  | H     | 255/557 (46%)    | 188 (74%)  | 55 (22%) | 12 (5%)  | 2           | 16  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 22  | I     | 206/233 (88%) | 196 (95%) | 9 (4%)   | 1 (0%)   | 24          | 63  |
| 23  | J     | 203/206 (98%) | 198 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 24  | K     | 154/167 (92%) | 146 (95%) | 7 (4%)   | 1 (1%)   | 21          | 58  |
| 25  | L     | 102/135 (76%) | 97 (95%)  | 4 (4%)   | 1 (1%)   | 12          | 47  |
| 26  | M     | 149/179 (83%) | 144 (97%) | 4 (3%)   | 1 (1%)   | 18          | 55  |
| 27  | N     | 127/130 (98%) | 121 (95%) | 5 (4%)   | 1 (1%)   | 16          | 53  |
| 28  | O     | 125/130 (96%) | 115 (92%) | 9 (7%)   | 1 (1%)   | 16          | 53  |
| 29  | P     | 97/103 (94%)  | 88 (91%)  | 8 (8%)   | 1 (1%)   | 12          | 47  |
| 30  | Q     | 115/129 (89%) | 104 (90%) | 9 (8%)   | 2 (2%)   | 7           | 34  |
| 31  | R     | 117/124 (94%) | 116 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 32  | S     | 98/101 (97%)  | 96 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 33  | T     | 86/89 (97%)   | 82 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 34  | U     | 80/82 (98%)   | 75 (94%)  | 4 (5%)   | 1 (1%)   | 9           | 40  |
| 35  | V     | 78/84 (93%)   | 74 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 36  | W     | 81/92 (88%)   | 78 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 37  | X     | 114/118 (97%) | 107 (94%) | 5 (4%)   | 2 (2%)   | 6           | 32  |
| 38  | Y     | 139/142 (98%) | 102 (73%) | 25 (18%) | 12 (9%)  | 0           | 8   |
| 39  | Z     | 28/121 (23%)  | 19 (68%)  | 7 (25%)  | 2 (7%)   | 1           | 10  |
| 41  | b     | 74/85 (87%)   | 69 (93%)  | 5 (7%)   | 0        | 100         | 100 |
| 42  | c     | 75/78 (96%)   | 72 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 44  | e     | 60/63 (95%)   | 57 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 45  | f     | 56/59 (95%)   | 53 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 46  | g     | 64/70 (91%)   | 63 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 47  | h     | 269/273 (98%) | 259 (96%) | 9 (3%)   | 1 (0%)   | 30          | 67  |
| 48  | i     | 54/57 (95%)   | 51 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 49  | j     | 207/209 (99%) | 198 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 50  | k     | 50/55 (91%)   | 50 (100%) | 0        | 0        | 100         | 100 |
| 51  | l     | 199/201 (99%) | 190 (96%) | 8 (4%)   | 1 (0%)   | 24          | 63  |
| 52  | m     | 44/46 (96%)   | 43 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 53  | n     | 175/179 (98%) | 162 (93%) | 11 (6%)  | 2 (1%)   | 11          | 45  |
| 54  | o     | 62/65 (95%)   | 59 (95%)  | 3 (5%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 55  | p     | 173/177 (98%)    | 161 (93%)  | 12 (7%)  | 0        | 100         | 100 |
| 56  | q     | 36/38 (95%)      | 35 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 57  | r     | 147/149 (99%)    | 136 (92%)  | 11 (8%)  | 0        | 100         | 100 |
| 58  | s     | 140/142 (99%)    | 135 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 59  | t     | 121/123 (98%)    | 111 (92%)  | 10 (8%)  | 0        | 100         | 100 |
| 60  | u     | 142/144 (99%)    | 135 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 61  | v     | 134/136 (98%)    | 129 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 62  | w     | 117/127 (92%)    | 107 (92%)  | 10 (8%)  | 0        | 100         | 100 |
| 63  | x     | 114/117 (97%)    | 108 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 64  | y     | 112/115 (97%)    | 105 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 65  | z     | 115/118 (98%)    | 110 (96%)  | 4 (4%)   | 1 (1%)   | 14          | 50  |
| All | All   | 9526/10577 (90%) | 8794 (92%) | 655 (7%) | 77 (1%)  | 18          | 53  |

All (77) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | 9     | 88  | HIS  |
| 11  | AA    | 913 | VAL  |
| 12  | AB    | 44  | VAL  |
| 12  | AB    | 49  | VAL  |
| 12  | AB    | 122 | PRO  |
| 21  | H     | 139 | ARG  |
| 21  | H     | 153 | GLU  |
| 21  | H     | 169 | SER  |
| 21  | H     | 306 | VAL  |
| 21  | H     | 340 | ARG  |
| 28  | O     | 56  | ASP  |
| 37  | X     | 103 | LYS  |
| 38  | Y     | 48  | ILE  |
| 9   | 9     | 33  | VAL  |
| 9   | 9     | 119 | PRO  |
| 12  | AB    | 50  | VAL  |
| 12  | AB    | 52  | ILE  |
| 14  | AE    | 92  | VAL  |
| 14  | AE    | 175 | GLU  |
| 21  | H     | 108 | VAL  |
| 21  | H     | 309 | MET  |
| 21  | H     | 333 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | Y     | 93  | ASN  |
| 47  | h     | 158 | ALA  |
| 51  | l     | 142 | ALA  |
| 65  | z     | 3   | ARG  |
| 9   | 9     | 48  | ALA  |
| 9   | 9     | 91  | ALA  |
| 9   | 9     | 118 | ILE  |
| 9   | 9     | 130 | PRO  |
| 11  | AA    | 893 | THR  |
| 12  | AB    | 59  | LYS  |
| 21  | H     | 76  | GLU  |
| 21  | H     | 142 | ARG  |
| 26  | M     | 130 | ASN  |
| 29  | P     | 58  | ASN  |
| 30  | Q     | 119 | ASN  |
| 38  | Y     | 20  | SER  |
| 38  | Y     | 64  | ARG  |
| 38  | Y     | 106 | GLN  |
| 9   | 9     | 69  | PHE  |
| 9   | 9     | 73  | LYS  |
| 9   | 9     | 108 | VAL  |
| 9   | 9     | 129 | LEU  |
| 9   | 9     | 133 | GLU  |
| 11  | AA    | 895 | LEU  |
| 12  | AB    | 45  | PRO  |
| 12  | AB    | 105 | ASP  |
| 13  | AC    | 193 | GLU  |
| 21  | H     | 82  | THR  |
| 22  | I     | 80  | LYS  |
| 37  | X     | 105 | ASN  |
| 38  | Y     | 83  | ALA  |
| 39  | Z     | 21  | GLU  |
| 53  | n     | 40  | VAL  |
| 14  | AE    | 74  | LYS  |
| 21  | H     | 70  | VAL  |
| 38  | Y     | 22  | PRO  |
| 38  | Y     | 71  | LYS  |
| 38  | Y     | 89  | SER  |
| 39  | Z     | 7   | ILE  |
| 4   | 3     | 39  | ILE  |
| 9   | 9     | 28  | ALA  |
| 13  | AC    | 192 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 38  | Y     | 62   | ALA  |
| 25  | L     | 96   | VAL  |
| 38  | Y     | 23   | VAL  |
| 38  | Y     | 100  | ILE  |
| 1   | 0     | 44   | GLY  |
| 12  | AB    | 162  | VAL  |
| 24  | K     | 44   | GLY  |
| 30  | Q     | 74   | VAL  |
| 34  | U     | 64   | GLY  |
| 9   | 9     | 54   | VAL  |
| 11  | AA    | 1317 | PRO  |
| 53  | n     | 62   | GLY  |
| 27  | N     | 75   | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 1   | 0     | 84/84 (100%)     | 76 (90%)   | 8 (10%)  | 8           | 26  |
| 2   | 1     | 93/93 (100%)     | 86 (92%)   | 7 (8%)   | 12          | 33  |
| 3   | 2     | 81/84 (96%)      | 77 (95%)   | 4 (5%)   | 22          | 44  |
| 4   | 3     | 84/85 (99%)      | 79 (94%)   | 5 (6%)   | 17          | 39  |
| 5   | 4     | 78/78 (100%)     | 75 (96%)   | 3 (4%)   | 29          | 51  |
| 9   | 9     | 112/123 (91%)    | 63 (56%)   | 49 (44%) | 0           | 0   |
| 11  | AA    | 1155/1157 (100%) | 1142 (99%) | 13 (1%)  | 65          | 74  |
| 12  | AB    | 150/158 (95%)    | 127 (85%)  | 23 (15%) | 3           | 13  |
| 13  | AC    | 186/286 (65%)    | 186 (100%) | 0        | 100         | 100 |
| 13  | AD    | 185/286 (65%)    | 185 (100%) | 0        | 100         | 100 |
| 14  | AE    | 1122/1168 (96%)  | 1107 (99%) | 15 (1%)  | 61          | 72  |
| 15  | AF    | 70/75 (93%)      | 69 (99%)   | 1 (1%)   | 59          | 72  |
| 16  | C     | 57/65 (88%)      | 55 (96%)   | 2 (4%)   | 32          | 53  |
| 18  | E     | 65/66 (98%)      | 61 (94%)   | 4 (6%)   | 16          | 38  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 19  | F     | 60/61 (98%)    | 57 (95%)  | 3 (5%)   | 22          | 43 |
| 20  | G     | 187/199 (94%)  | 174 (93%) | 13 (7%)  | 14          | 36 |
| 21  | H     | 137/461 (30%)  | 124 (90%) | 13 (10%) | 8           | 26 |
| 22  | I     | 171/190 (90%)  | 163 (95%) | 8 (5%)   | 23          | 45 |
| 23  | J     | 172/173 (99%)  | 164 (95%) | 8 (5%)   | 23          | 45 |
| 24  | K     | 119/126 (94%)  | 111 (93%) | 8 (7%)   | 15          | 37 |
| 25  | L     | 91/116 (78%)   | 84 (92%)  | 7 (8%)   | 12          | 32 |
| 26  | M     | 124/147 (84%)  | 113 (91%) | 11 (9%)  | 9           | 28 |
| 27  | N     | 104/105 (99%)  | 101 (97%) | 3 (3%)   | 37          | 58 |
| 28  | O     | 105/107 (98%)  | 99 (94%)  | 6 (6%)   | 18          | 40 |
| 29  | P     | 86/90 (96%)    | 77 (90%)  | 9 (10%)  | 6           | 22 |
| 30  | Q     | 90/99 (91%)    | 88 (98%)  | 2 (2%)   | 45          | 64 |
| 31  | R     | 101/104 (97%)  | 95 (94%)  | 6 (6%)   | 18          | 40 |
| 32  | S     | 83/84 (99%)    | 79 (95%)  | 4 (5%)   | 23          | 45 |
| 33  | T     | 76/77 (99%)    | 65 (86%)  | 11 (14%) | 3           | 14 |
| 34  | U     | 65/65 (100%)   | 60 (92%)  | 5 (8%)   | 12          | 32 |
| 35  | V     | 74/78 (95%)    | 71 (96%)  | 3 (4%)   | 27          | 49 |
| 36  | W     | 72/79 (91%)    | 66 (92%)  | 6 (8%)   | 10          | 30 |
| 37  | X     | 94/96 (98%)    | 87 (93%)  | 7 (7%)   | 13          | 34 |
| 38  | Y     | 109/110 (99%)  | 69 (63%)  | 40 (37%) | 0           | 1  |
| 39  | Z     | 26/85 (31%)    | 10 (38%)  | 16 (62%) | 0           | 0  |
| 41  | b     | 58/63 (92%)    | 57 (98%)  | 1 (2%)   | 53          | 68 |
| 42  | c     | 67/68 (98%)    | 64 (96%)  | 3 (4%)   | 24          | 46 |
| 44  | e     | 54/55 (98%)    | 51 (94%)  | 3 (6%)   | 19          | 41 |
| 45  | f     | 48/49 (98%)    | 43 (90%)  | 5 (10%)  | 7           | 22 |
| 46  | g     | 59/62 (95%)    | 54 (92%)  | 5 (8%)   | 10          | 29 |
| 47  | h     | 216/218 (99%)  | 199 (92%) | 17 (8%)  | 11          | 32 |
| 48  | i     | 47/48 (98%)    | 41 (87%)  | 6 (13%)  | 4           | 17 |
| 49  | j     | 164/164 (100%) | 156 (95%) | 8 (5%)   | 22          | 44 |
| 50  | k     | 47/49 (96%)    | 44 (94%)  | 3 (6%)   | 16          | 37 |
| 51  | l     | 165/165 (100%) | 151 (92%) | 14 (8%)  | 10          | 29 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 52  | m     | 38/38 (100%)    | 36 (95%)   | 2 (5%)   | 20          | 42 |
| 53  | n     | 148/150 (99%)   | 130 (88%)  | 18 (12%) | 5           | 18 |
| 54  | o     | 51/52 (98%)     | 47 (92%)   | 4 (8%)   | 11          | 32 |
| 55  | p     | 136/138 (99%)   | 130 (96%)  | 6 (4%)   | 25          | 47 |
| 56  | q     | 34/34 (100%)    | 31 (91%)   | 3 (9%)   | 9           | 29 |
| 57  | r     | 114/114 (100%)  | 102 (90%)  | 12 (10%) | 6           | 22 |
| 58  | s     | 116/116 (100%)  | 106 (91%)  | 10 (9%)  | 10          | 29 |
| 59  | t     | 104/104 (100%)  | 97 (93%)   | 7 (7%)   | 15          | 37 |
| 60  | u     | 103/103 (100%)  | 96 (93%)   | 7 (7%)   | 14          | 36 |
| 61  | v     | 109/109 (100%)  | 105 (96%)  | 4 (4%)   | 30          | 51 |
| 62  | w     | 99/103 (96%)    | 91 (92%)   | 8 (8%)   | 11          | 31 |
| 63  | x     | 86/87 (99%)     | 80 (93%)   | 6 (7%)   | 14          | 36 |
| 64  | y     | 99/100 (99%)    | 91 (92%)   | 8 (8%)   | 11          | 31 |
| 65  | z     | 89/90 (99%)     | 85 (96%)   | 4 (4%)   | 24          | 46 |
| All | All   | 7919/8739 (91%) | 7432 (94%) | 487 (6%) | 19          | 39 |

All (487) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 10  | LYS  |
| 1   | 0     | 38  | VAL  |
| 1   | 0     | 47  | VAL  |
| 1   | 0     | 48  | LYS  |
| 1   | 0     | 51  | VAL  |
| 1   | 0     | 68  | ARG  |
| 1   | 0     | 86  | GLN  |
| 1   | 0     | 96  | VAL  |
| 2   | 1     | 19  | LEU  |
| 2   | 1     | 30  | SER  |
| 2   | 1     | 41  | LYS  |
| 2   | 1     | 69  | LEU  |
| 2   | 1     | 97  | LEU  |
| 2   | 1     | 107 | VAL  |
| 2   | 1     | 110 | ARG  |
| 3   | 2     | 1   | MET  |
| 3   | 2     | 24  | MET  |
| 3   | 2     | 37  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2     | 93  | LEU  |
| 4   | 3     | 52  | LEU  |
| 4   | 3     | 70  | VAL  |
| 4   | 3     | 72  | ILE  |
| 4   | 3     | 99  | ASN  |
| 4   | 3     | 101 | GLU  |
| 5   | 4     | 40  | ILE  |
| 5   | 4     | 69  | GLU  |
| 5   | 4     | 71  | LYS  |
| 9   | 9     | 1   | MET  |
| 9   | 9     | 3   | LEU  |
| 9   | 9     | 4   | ASN  |
| 9   | 9     | 5   | LEU  |
| 9   | 9     | 6   | GLN  |
| 9   | 9     | 7   | ASP  |
| 9   | 9     | 11  | ILE  |
| 9   | 9     | 14  | GLU  |
| 9   | 9     | 23  | LEU  |
| 9   | 9     | 24  | SER  |
| 9   | 9     | 27  | VAL  |
| 9   | 9     | 31  | ARG  |
| 9   | 9     | 33  | VAL  |
| 9   | 9     | 34  | THR  |
| 9   | 9     | 35  | VAL  |
| 9   | 9     | 36  | ASP  |
| 9   | 9     | 37  | LYS  |
| 9   | 9     | 39  | THR  |
| 9   | 9     | 42  | ARG  |
| 9   | 9     | 43  | LYS  |
| 9   | 9     | 52  | MET  |
| 9   | 9     | 54  | VAL  |
| 9   | 9     | 55  | VAL  |
| 9   | 9     | 56  | ARG  |
| 9   | 9     | 57  | ASN  |
| 9   | 9     | 61  | ARG  |
| 9   | 9     | 69  | PHE  |
| 9   | 9     | 70  | GLU  |
| 9   | 9     | 71  | CYS  |
| 9   | 9     | 72  | LEU  |
| 9   | 9     | 73  | LYS  |
| 9   | 9     | 81  | LEU  |
| 9   | 9     | 86  | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | 9     | 94   | ARG  |
| 9   | 9     | 96   | PHE  |
| 9   | 9     | 98   | GLU  |
| 9   | 9     | 106  | PHE  |
| 9   | 9     | 107  | GLU  |
| 9   | 9     | 109  | LYS  |
| 9   | 9     | 113  | PHE  |
| 9   | 9     | 117  | LEU  |
| 9   | 9     | 122  | GLN  |
| 9   | 9     | 123  | ILE  |
| 9   | 9     | 125  | ARG  |
| 9   | 9     | 133  | GLU  |
| 9   | 9     | 134  | GLU  |
| 9   | 9     | 138  | ARG  |
| 9   | 9     | 142  | THR  |
| 9   | 9     | 143  | MET  |
| 11  | AA    | 145  | ILE  |
| 11  | AA    | 615  | VAL  |
| 11  | AA    | 892  | GLU  |
| 11  | AA    | 894  | GLN  |
| 11  | AA    | 895  | LEU  |
| 11  | AA    | 900  | LYS  |
| 11  | AA    | 903  | ARG  |
| 11  | AA    | 905  | ILE  |
| 11  | AA    | 909  | LYS  |
| 11  | AA    | 913  | VAL  |
| 11  | AA    | 914  | LYS  |
| 11  | AA    | 1076 | ILE  |
| 11  | AA    | 1151 | LEU  |
| 12  | AB    | 44   | VAL  |
| 12  | AB    | 46   | THR  |
| 12  | AB    | 47   | GLU  |
| 12  | AB    | 49   | VAL  |
| 12  | AB    | 52   | ILE  |
| 12  | AB    | 53   | ARG  |
| 12  | AB    | 57   | ARG  |
| 12  | AB    | 59   | LYS  |
| 12  | AB    | 62   | ARG  |
| 12  | AB    | 64   | PHE  |
| 12  | AB    | 65   | PHE  |
| 12  | AB    | 104  | SER  |
| 12  | AB    | 105  | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 12  | AB    | 106  | LYS  |
| 12  | AB    | 114  | ARG  |
| 12  | AB    | 127  | LEU  |
| 12  | AB    | 129  | GLU  |
| 12  | AB    | 159  | LYS  |
| 12  | AB    | 161  | SER  |
| 12  | AB    | 164  | ILE  |
| 12  | AB    | 165  | PHE  |
| 12  | AB    | 167  | ARG  |
| 12  | AB    | 169  | THR  |
| 14  | AE    | 69   | GLU  |
| 14  | AE    | 70   | CYS  |
| 14  | AE    | 71   | LEU  |
| 14  | AE    | 74   | LYS  |
| 14  | AE    | 76   | LYS  |
| 14  | AE    | 77   | ARG  |
| 14  | AE    | 78   | LEU  |
| 14  | AE    | 79   | LYS  |
| 14  | AE    | 81   | ARG  |
| 14  | AE    | 84   | ILE  |
| 14  | AE    | 85   | CYS  |
| 14  | AE    | 92   | VAL  |
| 14  | AE    | 93   | THR  |
| 14  | AE    | 514  | THR  |
| 14  | AE    | 1261 | LEU  |
| 15  | AF    | 63   | ILE  |
| 16  | C     | 33   | ILE  |
| 16  | C     | 74   | HIS  |
| 18  | E     | 6    | SER  |
| 18  | E     | 10   | ARG  |
| 18  | E     | 48   | GLN  |
| 18  | E     | 64   | LYS  |
| 19  | F     | 34   | ARG  |
| 19  | F     | 62   | ARG  |
| 19  | F     | 67   | ARG  |
| 20  | G     | 8    | ASP  |
| 20  | G     | 45   | LYS  |
| 20  | G     | 59   | LYS  |
| 20  | G     | 105  | LYS  |
| 20  | G     | 108  | ARG  |
| 20  | G     | 117  | LEU  |
| 20  | G     | 128  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | G     | 129 | LEU  |
| 20  | G     | 132 | LYS  |
| 20  | G     | 135 | LEU  |
| 20  | G     | 161 | LEU  |
| 20  | G     | 174 | LYS  |
| 20  | G     | 208 | ARG  |
| 21  | H     | 9   | PHE  |
| 21  | H     | 31  | ILE  |
| 21  | H     | 43  | LYS  |
| 21  | H     | 54  | LYS  |
| 21  | H     | 62  | ILE  |
| 21  | H     | 70  | VAL  |
| 21  | H     | 294 | VAL  |
| 21  | H     | 305 | HIS  |
| 21  | H     | 336 | ASP  |
| 21  | H     | 337 | GLU  |
| 21  | H     | 338 | GLU  |
| 21  | H     | 339 | ARG  |
| 21  | H     | 340 | ARG  |
| 22  | I     | 14  | ILE  |
| 22  | I     | 21  | THR  |
| 22  | I     | 33  | LEU  |
| 22  | I     | 75  | ILE  |
| 22  | I     | 89  | LYS  |
| 22  | I     | 175 | LEU  |
| 22  | I     | 178 | LEU  |
| 22  | I     | 200 | VAL  |
| 23  | J     | 47  | ARG  |
| 23  | J     | 48  | LEU  |
| 23  | J     | 95  | GLU  |
| 23  | J     | 104 | ARG  |
| 23  | J     | 105 | MET  |
| 23  | J     | 116 | GLN  |
| 23  | J     | 138 | SER  |
| 23  | J     | 143 | VAL  |
| 24  | K     | 10  | GLU  |
| 24  | K     | 15  | LEU  |
| 24  | K     | 60  | ILE  |
| 24  | K     | 114 | VAL  |
| 24  | K     | 115 | LEU  |
| 24  | K     | 138 | ARG  |
| 24  | K     | 141 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | K     | 162 | GLU  |
| 25  | L     | 7   | VAL  |
| 25  | L     | 16  | GLU  |
| 25  | L     | 24  | ARG  |
| 25  | L     | 36  | ILE  |
| 25  | L     | 38  | ARG  |
| 25  | L     | 54  | LEU  |
| 25  | L     | 86  | ARG  |
| 26  | M     | 7   | ILE  |
| 26  | M     | 17  | LYS  |
| 26  | M     | 21  | GLU  |
| 26  | M     | 23  | LEU  |
| 26  | M     | 27  | VAL  |
| 26  | M     | 50  | LEU  |
| 26  | M     | 79  | ARG  |
| 26  | M     | 91  | VAL  |
| 26  | M     | 109 | ARG  |
| 26  | M     | 130 | ASN  |
| 26  | M     | 146 | GLU  |
| 27  | N     | 96  | MET  |
| 27  | N     | 104 | VAL  |
| 27  | N     | 117 | ARG  |
| 28  | O     | 27  | LYS  |
| 28  | O     | 60  | LYS  |
| 28  | O     | 61  | LEU  |
| 28  | O     | 63  | LEU  |
| 28  | O     | 116 | VAL  |
| 28  | O     | 118 | LEU  |
| 29  | P     | 17  | LEU  |
| 29  | P     | 18  | ILE  |
| 29  | P     | 24  | GLU  |
| 29  | P     | 25  | ILE  |
| 29  | P     | 27  | GLU  |
| 29  | P     | 37  | ARG  |
| 29  | P     | 87  | LEU  |
| 29  | P     | 90  | LEU  |
| 29  | P     | 102 | LEU  |
| 30  | Q     | 15  | GLN  |
| 30  | Q     | 107 | ILE  |
| 31  | R     | 5   | ASN  |
| 31  | R     | 12  | ARG  |
| 31  | R     | 24  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | R     | 62  | GLU  |
| 31  | R     | 74  | LEU  |
| 31  | R     | 102 | LEU  |
| 32  | S     | 45  | VAL  |
| 32  | S     | 46  | LEU  |
| 32  | S     | 89  | MET  |
| 32  | S     | 92  | GLU  |
| 33  | T     | 10  | LYS  |
| 33  | T     | 22  | THR  |
| 33  | T     | 39  | LEU  |
| 33  | T     | 40  | GLN  |
| 33  | T     | 64  | ARG  |
| 33  | T     | 66  | LEU  |
| 33  | T     | 67  | LEU  |
| 33  | T     | 70  | LEU  |
| 33  | T     | 73  | LYS  |
| 33  | T     | 84  | ARG  |
| 33  | T     | 85  | LEU  |
| 34  | U     | 1   | MET  |
| 34  | U     | 2   | VAL  |
| 34  | U     | 6   | LEU  |
| 34  | U     | 19  | VAL  |
| 34  | U     | 50  | THR  |
| 35  | V     | 46  | VAL  |
| 35  | V     | 75  | LEU  |
| 35  | V     | 81  | LYS  |
| 36  | W     | 21  | LYS  |
| 36  | W     | 33  | THR  |
| 36  | W     | 49  | ILE  |
| 36  | W     | 58  | VAL  |
| 36  | W     | 79  | THR  |
| 36  | W     | 81  | ARG  |
| 37  | X     | 16  | VAL  |
| 37  | X     | 25  | VAL  |
| 37  | X     | 29  | ARG  |
| 37  | X     | 59  | GLU  |
| 37  | X     | 93  | ARG  |
| 37  | X     | 101 | ARG  |
| 37  | X     | 117 | LYS  |
| 38  | Y     | 4   | VAL  |
| 38  | Y     | 10  | LEU  |
| 38  | Y     | 16  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | Y     | 23  | VAL  |
| 38  | Y     | 27  | LEU  |
| 38  | Y     | 30  | GLN  |
| 38  | Y     | 36  | GLU  |
| 38  | Y     | 44  | LYS  |
| 38  | Y     | 45  | THR  |
| 38  | Y     | 48  | ILE  |
| 38  | Y     | 50  | LYS  |
| 38  | Y     | 52  | LEU  |
| 38  | Y     | 57  | VAL  |
| 38  | Y     | 58  | ILE  |
| 38  | Y     | 60  | VAL  |
| 38  | Y     | 61  | TYR  |
| 38  | Y     | 64  | ARG  |
| 38  | Y     | 65  | SER  |
| 38  | Y     | 67  | THR  |
| 38  | Y     | 71  | LYS  |
| 38  | Y     | 78  | LEU  |
| 38  | Y     | 80  | LYS  |
| 38  | Y     | 81  | LYS  |
| 38  | Y     | 91  | LYS  |
| 38  | Y     | 94  | LYS  |
| 38  | Y     | 95  | ASP  |
| 38  | Y     | 99  | LYS  |
| 38  | Y     | 100 | ILE  |
| 38  | Y     | 102 | ARG  |
| 38  | Y     | 104 | GLN  |
| 38  | Y     | 108 | ILE  |
| 38  | Y     | 112 | LYS  |
| 38  | Y     | 116 | MET  |
| 38  | Y     | 124 | MET  |
| 38  | Y     | 125 | THR  |
| 38  | Y     | 126 | ARG  |
| 38  | Y     | 133 | ARG  |
| 38  | Y     | 135 | MET  |
| 38  | Y     | 137 | LEU  |
| 38  | Y     | 138 | VAL  |
| 39  | Z     | 1   | SER  |
| 39  | Z     | 2   | ILE  |
| 39  | Z     | 3   | THR  |
| 39  | Z     | 4   | LYS  |
| 39  | Z     | 6   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | Z     | 7   | ILE  |
| 39  | Z     | 8   | ILE  |
| 39  | Z     | 14  | MET  |
| 39  | Z     | 16  | VAL  |
| 39  | Z     | 17  | MET  |
| 39  | Z     | 19  | VAL  |
| 39  | Z     | 23  | ILE  |
| 39  | Z     | 26  | MET  |
| 39  | Z     | 28  | GLU  |
| 39  | Z     | 29  | LYS  |
| 39  | Z     | 30  | PHE  |
| 41  | b     | 70  | GLU  |
| 42  | c     | 33  | LEU  |
| 42  | c     | 48  | THR  |
| 42  | c     | 71  | LEU  |
| 44  | e     | 18  | LEU  |
| 44  | e     | 58  | ASN  |
| 44  | e     | 60  | LYS  |
| 45  | f     | 3   | LYS  |
| 45  | f     | 11  | ARG  |
| 45  | f     | 25  | LEU  |
| 45  | f     | 45  | ARG  |
| 45  | f     | 55  | VAL  |
| 46  | g     | 3   | LYS  |
| 46  | g     | 16  | CYS  |
| 46  | g     | 24  | ILE  |
| 46  | g     | 36  | VAL  |
| 46  | g     | 47  | LYS  |
| 47  | h     | 51  | THR  |
| 47  | h     | 94  | VAL  |
| 47  | h     | 105 | LEU  |
| 47  | h     | 118 | SER  |
| 47  | h     | 125 | LYS  |
| 47  | h     | 130 | LEU  |
| 47  | h     | 141 | VAL  |
| 47  | h     | 156 | ARG  |
| 47  | h     | 183 | LYS  |
| 47  | h     | 187 | ASP  |
| 47  | h     | 195 | VAL  |
| 47  | h     | 202 | LEU  |
| 47  | h     | 203 | ARG  |
| 47  | h     | 204 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | h     | 205 | LEU  |
| 47  | h     | 242 | LYS  |
| 47  | h     | 271 | ARG  |
| 48  | i     | 9   | THR  |
| 48  | i     | 12  | LYS  |
| 48  | i     | 26  | THR  |
| 48  | i     | 27  | SER  |
| 48  | i     | 29  | SER  |
| 48  | i     | 40  | ARG  |
| 49  | j     | 13  | ARG  |
| 49  | j     | 18  | ASP  |
| 49  | j     | 91  | THR  |
| 49  | j     | 99  | GLU  |
| 49  | j     | 104 | VAL  |
| 49  | j     | 177 | VAL  |
| 49  | j     | 189 | VAL  |
| 49  | j     | 193 | VAL  |
| 50  | k     | 5   | ILE  |
| 50  | k     | 17  | THR  |
| 50  | k     | 24  | THR  |
| 51  | l     | 17  | THR  |
| 51  | l     | 22  | ASP  |
| 51  | l     | 40  | ARG  |
| 51  | l     | 48  | THR  |
| 51  | l     | 57  | LYS  |
| 51  | l     | 69  | ARG  |
| 51  | l     | 77  | ILE  |
| 51  | l     | 80  | SER  |
| 51  | l     | 108 | ILE  |
| 51  | l     | 109 | LEU  |
| 51  | l     | 111 | GLU  |
| 51  | l     | 122 | GLU  |
| 51  | l     | 149 | ILE  |
| 51  | l     | 179 | SER  |
| 52  | m     | 22  | MET  |
| 52  | m     | 42  | LEU  |
| 53  | n     | 6   | ASP  |
| 53  | n     | 10  | ASP  |
| 53  | n     | 26  | MET  |
| 53  | n     | 40  | VAL  |
| 53  | n     | 47  | LYS  |
| 53  | n     | 49  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | n     | 57  | LEU  |
| 53  | n     | 79  | ILE  |
| 53  | n     | 80  | ARG  |
| 53  | n     | 95  | ARG  |
| 53  | n     | 105 | THR  |
| 53  | n     | 117 | LEU  |
| 53  | n     | 122 | PHE  |
| 53  | n     | 123 | ASP  |
| 53  | n     | 132 | VAL  |
| 53  | n     | 140 | GLU  |
| 53  | n     | 141 | ILE  |
| 53  | n     | 163 | ASP  |
| 54  | o     | 8   | ARG  |
| 54  | o     | 30  | ARG  |
| 54  | o     | 31  | HIS  |
| 54  | o     | 55  | LEU  |
| 55  | p     | 11  | VAL  |
| 55  | p     | 85  | LYS  |
| 55  | p     | 95  | ARG  |
| 55  | p     | 125 | CYS  |
| 55  | p     | 168 | VAL  |
| 55  | p     | 171 | THR  |
| 56  | q     | 3   | VAL  |
| 56  | q     | 26  | ILE  |
| 56  | q     | 34  | LYS  |
| 57  | r     | 1   | MET  |
| 57  | r     | 9   | VAL  |
| 57  | r     | 11  | ASN  |
| 57  | r     | 12  | LEU  |
| 57  | r     | 15  | LEU  |
| 57  | r     | 41  | LYS  |
| 57  | r     | 66  | ASN  |
| 57  | r     | 72  | ILE  |
| 57  | r     | 76  | GLU  |
| 57  | r     | 94  | ILE  |
| 57  | r     | 101 | ASP  |
| 57  | r     | 127 | GLU  |
| 58  | s     | 1   | MET  |
| 58  | s     | 30  | THR  |
| 58  | s     | 31  | GLU  |
| 58  | s     | 43  | GLU  |
| 58  | s     | 57  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58  | s     | 123 | LYS  |
| 58  | s     | 124 | VAL  |
| 58  | s     | 139 | VAL  |
| 58  | s     | 140 | LEU  |
| 58  | s     | 142 | ILE  |
| 59  | t     | 7   | MET  |
| 59  | t     | 35  | VAL  |
| 59  | t     | 49  | ARG  |
| 59  | t     | 67  | LYS  |
| 59  | t     | 70  | ARG  |
| 59  | t     | 80  | ASP  |
| 59  | t     | 104 | THR  |
| 60  | u     | 5   | THR  |
| 60  | u     | 27  | LEU  |
| 60  | u     | 59  | ARG  |
| 60  | u     | 73  | ILE  |
| 60  | u     | 76  | GLU  |
| 60  | u     | 78  | ARG  |
| 60  | u     | 84  | LYS  |
| 61  | v     | 110 | GLU  |
| 61  | v     | 126 | ILE  |
| 61  | v     | 127 | LYS  |
| 61  | v     | 128 | THR  |
| 62  | w     | 2   | ARG  |
| 62  | w     | 20  | MET  |
| 62  | w     | 24  | MET  |
| 62  | w     | 51  | LEU  |
| 62  | w     | 65  | LEU  |
| 62  | w     | 69  | ARG  |
| 62  | w     | 95  | THR  |
| 62  | w     | 116 | VAL  |
| 63  | x     | 13  | ARG  |
| 63  | x     | 31  | THR  |
| 63  | x     | 47  | VAL  |
| 63  | x     | 48  | LEU  |
| 63  | x     | 91  | SER  |
| 63  | x     | 116 | GLN  |
| 64  | y     | 8   | LEU  |
| 64  | y     | 10  | GLN  |
| 64  | y     | 27  | GLU  |
| 64  | y     | 40  | LEU  |
| 64  | y     | 81  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 64  | y     | 85  | SER  |
| 64  | y     | 102 | GLU  |
| 64  | y     | 114 | LEU  |
| 65  | z     | 18  | LEU  |
| 65  | z     | 51  | ARG  |
| 65  | z     | 109 | LEU  |
| 65  | z     | 117 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 0     | 86   | GLN  |
| 2   | 1     | 61   | ASN  |
| 3   | 2     | 28   | ASN  |
| 3   | 2     | 59   | ASN  |
| 4   | 3     | 54   | GLN  |
| 9   | 9     | 103  | ASN  |
| 9   | 9     | 122  | GLN  |
| 11  | AA    | 69   | GLN  |
| 11  | AA    | 314  | ASN  |
| 11  | AA    | 330  | HIS  |
| 11  | AA    | 343  | HIS  |
| 11  | AA    | 513  | GLN  |
| 11  | AA    | 554  | HIS  |
| 11  | AA    | 580  | GLN  |
| 11  | AA    | 688  | GLN  |
| 11  | AA    | 762  | ASN  |
| 11  | AA    | 808  | ASN  |
| 11  | AA    | 1008 | GLN  |
| 11  | AA    | 1237 | HIS  |
| 11  | AA    | 1268 | GLN  |
| 11  | AA    | 1288 | GLN  |
| 11  | AA    | 1313 | HIS  |
| 13  | AD    | 37   | HIS  |
| 13  | AD    | 66   | HIS  |
| 13  | AD    | 84   | ASN  |
| 13  | AD    | 117  | HIS  |
| 13  | AD    | 128  | HIS  |
| 13  | AD    | 227  | GLN  |
| 14  | AE    | 80   | HIS  |
| 14  | AE    | 157  | GLN  |
| 14  | AE    | 164  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 14  | AE    | 232  | ASN  |
| 14  | AE    | 365  | GLN  |
| 14  | AE    | 450  | HIS  |
| 14  | AE    | 469  | HIS  |
| 14  | AE    | 777  | HIS  |
| 14  | AE    | 865  | HIS  |
| 14  | AE    | 910  | ASN  |
| 14  | AE    | 1108 | GLN  |
| 14  | AE    | 1197 | ASN  |
| 14  | AE    | 1235 | ASN  |
| 14  | AE    | 1238 | GLN  |
| 14  | AE    | 1326 | GLN  |
| 15  | AF    | 31   | GLN  |
| 15  | AF    | 62   | GLN  |
| 18  | E     | 3    | ASN  |
| 18  | E     | 55   | GLN  |
| 18  | E     | 61   | GLN  |
| 20  | G     | 18   | HIS  |
| 20  | G     | 58   | ASN  |
| 20  | G     | 94   | HIS  |
| 22  | I     | 6    | HIS  |
| 22  | I     | 25   | ASN  |
| 22  | I     | 123  | GLN  |
| 23  | J     | 36   | GLN  |
| 23  | J     | 40   | GLN  |
| 23  | J     | 41   | HIS  |
| 24  | K     | 97   | GLN  |
| 25  | L     | 11   | HIS  |
| 25  | L     | 46   | GLN  |
| 25  | L     | 63   | ASN  |
| 25  | L     | 94   | HIS  |
| 26  | M     | 97   | ASN  |
| 26  | M     | 148  | ASN  |
| 28  | O     | 81   | HIS  |
| 28  | O     | 126  | GLN  |
| 29  | P     | 58   | ASN  |
| 31  | R     | 72   | HIS  |
| 32  | S     | 60   | GLN  |
| 33  | T     | 40   | GLN  |
| 34  | U     | 59   | HIS  |
| 37  | X     | 105  | ASN  |
| 46  | g     | 33   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | g     | 41  | HIS  |
| 47  | h     | 70  | ASN  |
| 48  | i     | 5   | GLN  |
| 50  | k     | 26  | ASN  |
| 53  | n     | 63  | GLN  |
| 54  | o     | 28  | ASN  |
| 55  | p     | 88  | GLN  |
| 57  | r     | 20  | ASN  |
| 57  | r     | 133 | GLN  |
| 59  | t     | 88  | ASN  |
| 64  | y     | 15  | GLN  |
| 64  | y     | 66  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 10  | A     | 75/76 (98%)     | 29 (38%)          | 6 (8%)          |
| 10  | B     | 75/76 (98%)     | 35 (46%)          | 6 (8%)          |
| 17  | D     | 1515/1542 (98%) | 290 (19%)         | 35 (2%)         |
| 40  | a     | 2859/2904 (98%) | 540 (18%)         | 0               |
| 43  | d     | 119/120 (99%)   | 17 (14%)          | 0               |
| 8   | 7     | 33/45 (73%)     | 20 (60%)          | 5 (15%)         |
| All | All   | 4676/4763 (98%) | 931 (19%)         | 52 (1%)         |

All (931) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 7     | -18 | G    |
| 8   | 7     | -17 | U    |
| 8   | 7     | -16 | U    |
| 8   | 7     | -14 | U    |
| 8   | 7     | -13 | U    |
| 8   | 7     | -12 | U    |
| 8   | 7     | -11 | U    |
| 8   | 7     | -10 | U    |
| 8   | 7     | -9  | U    |
| 8   | 7     | -8  | U    |
| 8   | 7     | -7  | U    |
| 8   | 7     | -6  | U    |
| 8   | 7     | -5  | U    |
| 8   | 7     | -4  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 7     | -3  | U    |
| 8   | 7     | -2  | U    |
| 8   | 7     | 0   | U    |
| 8   | 7     | 1   | U    |
| 8   | 7     | 12  | G    |
| 8   | 7     | 13  | G    |
| 10  | A     | 2   | G    |
| 10  | A     | 6   | G    |
| 10  | A     | 7   | G    |
| 10  | A     | 8   | U    |
| 10  | A     | 10  | G    |
| 10  | A     | 13  | C    |
| 10  | A     | 14  | A    |
| 10  | A     | 15  | G    |
| 10  | A     | 16  | C    |
| 10  | A     | 17  | C    |
| 10  | A     | 18  | G    |
| 10  | A     | 19  | G    |
| 10  | A     | 20  | U    |
| 10  | A     | 21  | A    |
| 10  | A     | 22  | G    |
| 10  | A     | 23  | C    |
| 10  | A     | 46  | G    |
| 10  | A     | 47  | U    |
| 10  | A     | 48  | C    |
| 10  | A     | 49  | G    |
| 10  | A     | 52  | G    |
| 10  | A     | 57  | A    |
| 10  | A     | 58  | A    |
| 10  | A     | 59  | A    |
| 10  | A     | 61  | C    |
| 10  | A     | 66  | C    |
| 10  | A     | 69  | C    |
| 10  | A     | 71  | C    |
| 10  | A     | 73  | A    |
| 10  | B     | 2   | G    |
| 10  | B     | 6   | G    |
| 10  | B     | 7   | G    |
| 10  | B     | 8   | U    |
| 10  | B     | 10  | G    |
| 10  | B     | 13  | C    |
| 10  | B     | 14  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | B     | 15  | G    |
| 10  | B     | 16  | C    |
| 10  | B     | 17  | C    |
| 10  | B     | 18  | G    |
| 10  | B     | 19  | G    |
| 10  | B     | 20  | U    |
| 10  | B     | 21  | A    |
| 10  | B     | 22  | G    |
| 10  | B     | 23  | C    |
| 10  | B     | 30  | G    |
| 10  | B     | 31  | G    |
| 10  | B     | 32  | C    |
| 10  | B     | 36  | U    |
| 10  | B     | 37  | A    |
| 10  | B     | 38  | A    |
| 10  | B     | 46  | G    |
| 10  | B     | 47  | U    |
| 10  | B     | 48  | C    |
| 10  | B     | 49  | G    |
| 10  | B     | 52  | G    |
| 10  | B     | 57  | A    |
| 10  | B     | 58  | A    |
| 10  | B     | 59  | A    |
| 10  | B     | 61  | C    |
| 10  | B     | 66  | C    |
| 10  | B     | 69  | C    |
| 10  | B     | 71  | C    |
| 10  | B     | 73  | A    |
| 17  | D     | 4   | U    |
| 17  | D     | 5   | U    |
| 17  | D     | 9   | G    |
| 17  | D     | 22  | G    |
| 17  | D     | 29  | U    |
| 17  | D     | 32  | A    |
| 17  | D     | 39  | G    |
| 17  | D     | 41  | G    |
| 17  | D     | 47  | C    |
| 17  | D     | 48  | C    |
| 17  | D     | 50  | A    |
| 17  | D     | 51  | A    |
| 17  | D     | 52  | C    |
| 17  | D     | 54  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | D     | 69  | G    |
| 17  | D     | 70  | U    |
| 17  | D     | 71  | A    |
| 17  | D     | 72  | A    |
| 17  | D     | 74  | A    |
| 17  | D     | 76  | G    |
| 17  | D     | 82  | G    |
| 17  | D     | 83  | C    |
| 17  | D     | 84  | U    |
| 17  | D     | 87  | C    |
| 17  | D     | 90  | C    |
| 17  | D     | 94  | G    |
| 17  | D     | 95  | C    |
| 17  | D     | 96  | U    |
| 17  | D     | 108 | G    |
| 17  | D     | 120 | A    |
| 17  | D     | 122 | G    |
| 17  | D     | 128 | G    |
| 17  | D     | 131 | A    |
| 17  | D     | 141 | G    |
| 17  | D     | 144 | G    |
| 17  | D     | 148 | G    |
| 17  | D     | 149 | A    |
| 17  | D     | 160 | A    |
| 17  | D     | 164 | G    |
| 17  | D     | 173 | U    |
| 17  | D     | 181 | A    |
| 17  | D     | 182 | A    |
| 17  | D     | 197 | A    |
| 17  | D     | 198 | G    |
| 17  | D     | 204 | G    |
| 17  | D     | 208 | U    |
| 17  | D     | 209 | U    |
| 17  | D     | 210 | C    |
| 17  | D     | 211 | G    |
| 17  | D     | 212 | G    |
| 17  | D     | 216 | U    |
| 17  | D     | 226 | G    |
| 17  | D     | 245 | U    |
| 17  | D     | 247 | G    |
| 17  | D     | 251 | G    |
| 17  | D     | 253 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | D     | 258 | G    |
| 17  | D     | 262 | A    |
| 17  | D     | 266 | G    |
| 17  | D     | 267 | C    |
| 17  | D     | 271 | C    |
| 17  | D     | 279 | A    |
| 17  | D     | 289 | G    |
| 17  | D     | 299 | G    |
| 17  | D     | 306 | A    |
| 17  | D     | 321 | A    |
| 17  | D     | 328 | C    |
| 17  | D     | 329 | A    |
| 17  | D     | 332 | G    |
| 17  | D     | 347 | G    |
| 17  | D     | 352 | C    |
| 17  | D     | 353 | A    |
| 17  | D     | 354 | G    |
| 17  | D     | 355 | C    |
| 17  | D     | 367 | U    |
| 17  | D     | 372 | C    |
| 17  | D     | 373 | A    |
| 17  | D     | 376 | G    |
| 17  | D     | 382 | A    |
| 17  | D     | 384 | G    |
| 17  | D     | 392 | C    |
| 17  | D     | 393 | A    |
| 17  | D     | 397 | A    |
| 17  | D     | 406 | G    |
| 17  | D     | 412 | A    |
| 17  | D     | 413 | G    |
| 17  | D     | 414 | A    |
| 17  | D     | 421 | U    |
| 17  | D     | 422 | C    |
| 17  | D     | 424 | G    |
| 17  | D     | 429 | U    |
| 17  | D     | 446 | G    |
| 17  | D     | 451 | A    |
| 17  | D     | 457 | G    |
| 17  | D     | 458 | U    |
| 17  | D     | 460 | A    |
| 17  | D     | 463 | U    |
| 17  | D     | 464 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | D     | 467 | U    |
| 17  | D     | 468 | A    |
| 17  | D     | 469 | C    |
| 17  | D     | 478 | A    |
| 17  | D     | 479 | U    |
| 17  | D     | 481 | G    |
| 17  | D     | 484 | G    |
| 17  | D     | 485 | U    |
| 17  | D     | 486 | U    |
| 17  | D     | 505 | G    |
| 17  | D     | 509 | A    |
| 17  | D     | 511 | C    |
| 17  | D     | 518 | C    |
| 17  | D     | 519 | C    |
| 17  | D     | 526 | C    |
| 17  | D     | 531 | U    |
| 17  | D     | 532 | A    |
| 17  | D     | 533 | A    |
| 17  | D     | 542 | G    |
| 17  | D     | 547 | A    |
| 17  | D     | 559 | A    |
| 17  | D     | 562 | U    |
| 17  | D     | 568 | G    |
| 17  | D     | 572 | A    |
| 17  | D     | 573 | A    |
| 17  | D     | 576 | C    |
| 17  | D     | 577 | G    |
| 17  | D     | 579 | A    |
| 17  | D     | 596 | A    |
| 17  | D     | 628 | G    |
| 17  | D     | 633 | G    |
| 17  | D     | 641 | U    |
| 17  | D     | 642 | A    |
| 17  | D     | 649 | A    |
| 17  | D     | 650 | G    |
| 17  | D     | 653 | U    |
| 17  | D     | 665 | A    |
| 17  | D     | 666 | G    |
| 17  | D     | 687 | A    |
| 17  | D     | 700 | G    |
| 17  | D     | 723 | U    |
| 17  | D     | 724 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 17  | D     | 731  | G    |
| 17  | D     | 734  | G    |
| 17  | D     | 747  | A    |
| 17  | D     | 748  | G    |
| 17  | D     | 755  | G    |
| 17  | D     | 760  | G    |
| 17  | D     | 777  | A    |
| 17  | D     | 793  | U    |
| 17  | D     | 794  | A    |
| 17  | D     | 815  | A    |
| 17  | D     | 817  | C    |
| 17  | D     | 828  | U    |
| 17  | D     | 829  | G    |
| 17  | D     | 832  | G    |
| 17  | D     | 841  | C    |
| 17  | D     | 844  | G    |
| 17  | D     | 845  | A    |
| 17  | D     | 849  | G    |
| 17  | D     | 874  | G    |
| 17  | D     | 887  | G    |
| 17  | D     | 902  | G    |
| 17  | D     | 914  | A    |
| 17  | D     | 916  | U    |
| 17  | D     | 926  | G    |
| 17  | D     | 934  | C    |
| 17  | D     | 935  | A    |
| 17  | D     | 954  | G    |
| 17  | D     | 960  | U    |
| 17  | D     | 963  | G    |
| 17  | D     | 969  | A    |
| 17  | D     | 972  | C    |
| 17  | D     | 975  | A    |
| 17  | D     | 976  | G    |
| 17  | D     | 991  | U    |
| 17  | D     | 992  | U    |
| 17  | D     | 993  | G    |
| 17  | D     | 996  | A    |
| 17  | D     | 999  | C    |
| 17  | D     | 1004 | A    |
| 17  | D     | 1008 | U    |
| 17  | D     | 1009 | U    |
| 17  | D     | 1017 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 17  | D     | 1018 | G    |
| 17  | D     | 1021 | A    |
| 17  | D     | 1024 | G    |
| 17  | D     | 1026 | G    |
| 17  | D     | 1028 | C    |
| 17  | D     | 1030 | U    |
| 17  | D     | 1031 | C    |
| 17  | D     | 1037 | C    |
| 17  | D     | 1043 | G    |
| 17  | D     | 1044 | A    |
| 17  | D     | 1046 | A    |
| 17  | D     | 1065 | U    |
| 17  | D     | 1085 | U    |
| 17  | D     | 1086 | U    |
| 17  | D     | 1094 | G    |
| 17  | D     | 1095 | U    |
| 17  | D     | 1099 | G    |
| 17  | D     | 1101 | A    |
| 17  | D     | 1124 | G    |
| 17  | D     | 1133 | G    |
| 17  | D     | 1135 | U    |
| 17  | D     | 1136 | C    |
| 17  | D     | 1137 | C    |
| 17  | D     | 1139 | G    |
| 17  | D     | 1140 | C    |
| 17  | D     | 1141 | C    |
| 17  | D     | 1142 | G    |
| 17  | D     | 1143 | G    |
| 17  | D     | 1145 | A    |
| 17  | D     | 1146 | A    |
| 17  | D     | 1151 | A    |
| 17  | D     | 1152 | A    |
| 17  | D     | 1158 | C    |
| 17  | D     | 1159 | U    |
| 17  | D     | 1167 | A    |
| 17  | D     | 1171 | A    |
| 17  | D     | 1174 | G    |
| 17  | D     | 1175 | G    |
| 17  | D     | 1176 | A    |
| 17  | D     | 1184 | G    |
| 17  | D     | 1196 | A    |
| 17  | D     | 1197 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 17  | D     | 1206 | G    |
| 17  | D     | 1211 | U    |
| 17  | D     | 1212 | U    |
| 17  | D     | 1213 | A    |
| 17  | D     | 1214 | C    |
| 17  | D     | 1215 | G    |
| 17  | D     | 1226 | C    |
| 17  | D     | 1227 | A    |
| 17  | D     | 1228 | C    |
| 17  | D     | 1238 | A    |
| 17  | D     | 1256 | A    |
| 17  | D     | 1257 | A    |
| 17  | D     | 1260 | G    |
| 17  | D     | 1275 | A    |
| 17  | D     | 1276 | G    |
| 17  | D     | 1278 | G    |
| 17  | D     | 1279 | G    |
| 17  | D     | 1280 | A    |
| 17  | D     | 1285 | A    |
| 17  | D     | 1286 | U    |
| 17  | D     | 1287 | A    |
| 17  | D     | 1299 | A    |
| 17  | D     | 1300 | G    |
| 17  | D     | 1302 | C    |
| 17  | D     | 1305 | G    |
| 17  | D     | 1312 | G    |
| 17  | D     | 1317 | C    |
| 17  | D     | 1320 | C    |
| 17  | D     | 1323 | G    |
| 17  | D     | 1329 | A    |
| 17  | D     | 1338 | G    |
| 17  | D     | 1340 | A    |
| 17  | D     | 1346 | A    |
| 17  | D     | 1347 | G    |
| 17  | D     | 1353 | G    |
| 17  | D     | 1363 | A    |
| 17  | D     | 1370 | G    |
| 17  | D     | 1378 | C    |
| 17  | D     | 1379 | G    |
| 17  | D     | 1381 | U    |
| 17  | D     | 1391 | U    |
| 17  | D     | 1396 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 17  | D     | 1397 | C    |
| 17  | D     | 1398 | A    |
| 17  | D     | 1404 | C    |
| 17  | D     | 1419 | G    |
| 17  | D     | 1429 | A    |
| 17  | D     | 1441 | A    |
| 17  | D     | 1446 | A    |
| 17  | D     | 1447 | A    |
| 17  | D     | 1448 | C    |
| 17  | D     | 1452 | C    |
| 17  | D     | 1453 | G    |
| 17  | D     | 1475 | G    |
| 17  | D     | 1487 | G    |
| 17  | D     | 1492 | A    |
| 17  | D     | 1493 | A    |
| 17  | D     | 1494 | G    |
| 17  | D     | 1495 | U    |
| 17  | D     | 1497 | G    |
| 17  | D     | 1503 | A    |
| 17  | D     | 1506 | U    |
| 17  | D     | 1517 | G    |
| 17  | D     | 1529 | G    |
| 17  | D     | 1530 | G    |
| 17  | D     | 1534 | A    |
| 40  | a     | 10   | A    |
| 40  | a     | 15   | G    |
| 40  | a     | 34   | U    |
| 40  | a     | 35   | G    |
| 40  | a     | 46   | G    |
| 40  | a     | 58   | G    |
| 40  | a     | 60   | G    |
| 40  | a     | 63   | A    |
| 40  | a     | 71   | A    |
| 40  | a     | 74   | A    |
| 40  | a     | 75   | G    |
| 40  | a     | 83   | A    |
| 40  | a     | 84   | A    |
| 40  | a     | 85   | G    |
| 40  | a     | 93   | G    |
| 40  | a     | 96   | C    |
| 40  | a     | 102  | U    |
| 40  | a     | 103  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | a     | 110 | G    |
| 40  | a     | 114 | U    |
| 40  | a     | 118 | A    |
| 40  | a     | 119 | A    |
| 40  | a     | 120 | U    |
| 40  | a     | 122 | G    |
| 40  | a     | 131 | A    |
| 40  | a     | 136 | G    |
| 40  | a     | 139 | U    |
| 40  | a     | 140 | C    |
| 40  | a     | 141 | G    |
| 40  | a     | 145 | C    |
| 40  | a     | 163 | C    |
| 40  | a     | 165 | A    |
| 40  | a     | 181 | A    |
| 40  | a     | 196 | A    |
| 40  | a     | 199 | A    |
| 40  | a     | 200 | U    |
| 40  | a     | 215 | G    |
| 40  | a     | 216 | A    |
| 40  | a     | 222 | A    |
| 40  | a     | 225 | C    |
| 40  | a     | 248 | G    |
| 40  | a     | 249 | C    |
| 40  | a     | 261 | G    |
| 40  | a     | 264 | C    |
| 40  | a     | 265 | A    |
| 40  | a     | 266 | G    |
| 40  | a     | 267 | C    |
| 40  | a     | 271 | G    |
| 40  | a     | 272 | A    |
| 40  | a     | 275 | C    |
| 40  | a     | 276 | U    |
| 40  | a     | 278 | A    |
| 40  | a     | 285 | G    |
| 40  | a     | 311 | A    |
| 40  | a     | 324 | A    |
| 40  | a     | 329 | G    |
| 40  | a     | 330 | A    |
| 40  | a     | 353 | C    |
| 40  | a     | 359 | G    |
| 40  | a     | 361 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | a     | 362 | A    |
| 40  | a     | 371 | A    |
| 40  | a     | 372 | G    |
| 40  | a     | 373 | U    |
| 40  | a     | 375 | G    |
| 40  | a     | 383 | C    |
| 40  | a     | 386 | G    |
| 40  | a     | 396 | G    |
| 40  | a     | 405 | U    |
| 40  | a     | 411 | G    |
| 40  | a     | 412 | A    |
| 40  | a     | 420 | C    |
| 40  | a     | 424 | G    |
| 40  | a     | 435 | C    |
| 40  | a     | 451 | U    |
| 40  | a     | 456 | C    |
| 40  | a     | 457 | A    |
| 40  | a     | 477 | A    |
| 40  | a     | 481 | G    |
| 40  | a     | 491 | G    |
| 40  | a     | 501 | A    |
| 40  | a     | 503 | A    |
| 40  | a     | 504 | A    |
| 40  | a     | 505 | A    |
| 40  | a     | 509 | C    |
| 40  | a     | 522 | A    |
| 40  | a     | 529 | A    |
| 40  | a     | 532 | A    |
| 40  | a     | 543 | G    |
| 40  | a     | 546 | U    |
| 40  | a     | 547 | A    |
| 40  | a     | 548 | G    |
| 40  | a     | 549 | G    |
| 40  | a     | 551 | G    |
| 40  | a     | 563 | A    |
| 40  | a     | 569 | U    |
| 40  | a     | 573 | U    |
| 40  | a     | 575 | A    |
| 40  | a     | 588 | U    |
| 40  | a     | 603 | A    |
| 40  | a     | 609 | A    |
| 40  | a     | 613 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | a     | 614 | A    |
| 40  | a     | 615 | U    |
| 40  | a     | 616 | A    |
| 40  | a     | 618 | G    |
| 40  | a     | 620 | G    |
| 40  | a     | 621 | A    |
| 40  | a     | 627 | A    |
| 40  | a     | 637 | A    |
| 40  | a     | 645 | C    |
| 40  | a     | 647 | G    |
| 40  | a     | 654 | A    |
| 40  | a     | 664 | G    |
| 40  | a     | 668 | A    |
| 40  | a     | 685 | A    |
| 40  | a     | 686 | U    |
| 40  | a     | 710 | U    |
| 40  | a     | 717 | C    |
| 40  | a     | 730 | A    |
| 40  | a     | 738 | G    |
| 40  | a     | 757 | G    |
| 40  | a     | 764 | A    |
| 40  | a     | 765 | C    |
| 40  | a     | 775 | G    |
| 40  | a     | 776 | G    |
| 40  | a     | 782 | A    |
| 40  | a     | 784 | G    |
| 40  | a     | 785 | G    |
| 40  | a     | 800 | A    |
| 40  | a     | 802 | A    |
| 40  | a     | 805 | G    |
| 40  | a     | 812 | C    |
| 40  | a     | 819 | A    |
| 40  | a     | 827 | U    |
| 40  | a     | 828 | U    |
| 40  | a     | 845 | A    |
| 40  | a     | 846 | U    |
| 40  | a     | 858 | G    |
| 40  | a     | 859 | G    |
| 40  | a     | 869 | G    |
| 40  | a     | 878 | A    |
| 40  | a     | 881 | G    |
| 40  | a     | 883 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 884  | U    |
| 40  | a     | 885  | C    |
| 40  | a     | 888  | C    |
| 40  | a     | 891  | G    |
| 40  | a     | 892  | A    |
| 40  | a     | 893  | C    |
| 40  | a     | 895  | U    |
| 40  | a     | 896  | A    |
| 40  | a     | 897  | C    |
| 40  | a     | 899  | A    |
| 40  | a     | 907  | G    |
| 40  | a     | 910  | A    |
| 40  | a     | 914  | G    |
| 40  | a     | 915  | C    |
| 40  | a     | 931  | U    |
| 40  | a     | 941  | A    |
| 40  | a     | 945  | A    |
| 40  | a     | 946  | C    |
| 40  | a     | 953  | G    |
| 40  | a     | 961  | C    |
| 40  | a     | 974  | G    |
| 40  | a     | 983  | A    |
| 40  | a     | 984  | A    |
| 40  | a     | 985  | C    |
| 40  | a     | 995  | C    |
| 40  | a     | 996  | A    |
| 40  | a     | 999  | U    |
| 40  | a     | 1005 | C    |
| 40  | a     | 1012 | U    |
| 40  | a     | 1013 | C    |
| 40  | a     | 1022 | G    |
| 40  | a     | 1023 | U    |
| 40  | a     | 1026 | G    |
| 40  | a     | 1033 | U    |
| 40  | a     | 1041 | G    |
| 40  | a     | 1042 | G    |
| 40  | a     | 1045 | C    |
| 40  | a     | 1046 | A    |
| 40  | a     | 1047 | G    |
| 40  | a     | 1060 | U    |
| 40  | a     | 1061 | U    |
| 40  | a     | 1062 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 1063 | G    |
| 40  | a     | 1064 | C    |
| 40  | a     | 1065 | U    |
| 40  | a     | 1066 | U    |
| 40  | a     | 1067 | A    |
| 40  | a     | 1068 | G    |
| 40  | a     | 1069 | A    |
| 40  | a     | 1070 | A    |
| 40  | a     | 1071 | G    |
| 40  | a     | 1073 | A    |
| 40  | a     | 1074 | G    |
| 40  | a     | 1076 | C    |
| 40  | a     | 1079 | C    |
| 40  | a     | 1080 | A    |
| 40  | a     | 1081 | U    |
| 40  | a     | 1082 | U    |
| 40  | a     | 1083 | U    |
| 40  | a     | 1084 | A    |
| 40  | a     | 1087 | G    |
| 40  | a     | 1088 | A    |
| 40  | a     | 1090 | A    |
| 40  | a     | 1095 | A    |
| 40  | a     | 1096 | A    |
| 40  | a     | 1107 | G    |
| 40  | a     | 1110 | G    |
| 40  | a     | 1111 | A    |
| 40  | a     | 1112 | G    |
| 40  | a     | 1119 | U    |
| 40  | a     | 1122 | G    |
| 40  | a     | 1132 | U    |
| 40  | a     | 1134 | A    |
| 40  | a     | 1135 | C    |
| 40  | a     | 1142 | A    |
| 40  | a     | 1143 | A    |
| 40  | a     | 1169 | A    |
| 40  | a     | 1170 | C    |
| 40  | a     | 1173 | U    |
| 40  | a     | 1174 | U    |
| 40  | a     | 1175 | A    |
| 40  | a     | 1176 | U    |
| 40  | a     | 1177 | G    |
| 40  | a     | 1178 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 1179 | G    |
| 40  | a     | 1180 | U    |
| 40  | a     | 1186 | G    |
| 40  | a     | 1238 | G    |
| 40  | a     | 1248 | G    |
| 40  | a     | 1253 | A    |
| 40  | a     | 1256 | G    |
| 40  | a     | 1266 | G    |
| 40  | a     | 1271 | G    |
| 40  | a     | 1272 | A    |
| 40  | a     | 1273 | U    |
| 40  | a     | 1301 | A    |
| 40  | a     | 1321 | A    |
| 40  | a     | 1345 | C    |
| 40  | a     | 1352 | U    |
| 40  | a     | 1365 | A    |
| 40  | a     | 1368 | G    |
| 40  | a     | 1378 | A    |
| 40  | a     | 1379 | U    |
| 40  | a     | 1380 | G    |
| 40  | a     | 1383 | A    |
| 40  | a     | 1387 | A    |
| 40  | a     | 1395 | A    |
| 40  | a     | 1406 | U    |
| 40  | a     | 1407 | G    |
| 40  | a     | 1408 | G    |
| 40  | a     | 1411 | U    |
| 40  | a     | 1414 | C    |
| 40  | a     | 1415 | U    |
| 40  | a     | 1416 | G    |
| 40  | a     | 1417 | C    |
| 40  | a     | 1419 | A    |
| 40  | a     | 1420 | A    |
| 40  | a     | 1428 | C    |
| 40  | a     | 1452 | G    |
| 40  | a     | 1453 | A    |
| 40  | a     | 1460 | U    |
| 40  | a     | 1478 | G    |
| 40  | a     | 1482 | G    |
| 40  | a     | 1490 | A    |
| 40  | a     | 1491 | G    |
| 40  | a     | 1497 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 1503 | A    |
| 40  | a     | 1508 | A    |
| 40  | a     | 1509 | A    |
| 40  | a     | 1510 | G    |
| 40  | a     | 1515 | A    |
| 40  | a     | 1529 | G    |
| 40  | a     | 1534 | U    |
| 40  | a     | 1535 | A    |
| 40  | a     | 1536 | C    |
| 40  | a     | 1537 | G    |
| 40  | a     | 1554 | U    |
| 40  | a     | 1559 | U    |
| 40  | a     | 1566 | A    |
| 40  | a     | 1569 | A    |
| 40  | a     | 1578 | U    |
| 40  | a     | 1580 | A    |
| 40  | a     | 1581 | G    |
| 40  | a     | 1582 | C    |
| 40  | a     | 1583 | A    |
| 40  | a     | 1584 | U    |
| 40  | a     | 1589 | U    |
| 40  | a     | 1590 | A    |
| 40  | a     | 1608 | A    |
| 40  | a     | 1609 | A    |
| 40  | a     | 1610 | A    |
| 40  | a     | 1647 | U    |
| 40  | a     | 1648 | U    |
| 40  | a     | 1649 | G    |
| 40  | a     | 1651 | G    |
| 40  | a     | 1674 | G    |
| 40  | a     | 1677 | A    |
| 40  | a     | 1703 | G    |
| 40  | a     | 1714 | U    |
| 40  | a     | 1715 | G    |
| 40  | a     | 1718 | G    |
| 40  | a     | 1729 | U    |
| 40  | a     | 1730 | C    |
| 40  | a     | 1732 | C    |
| 40  | a     | 1738 | G    |
| 40  | a     | 1750 | G    |
| 40  | a     | 1755 | A    |
| 40  | a     | 1758 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 1764 | C    |
| 40  | a     | 1773 | A    |
| 40  | a     | 1791 | A    |
| 40  | a     | 1800 | C    |
| 40  | a     | 1801 | A    |
| 40  | a     | 1808 | A    |
| 40  | a     | 1811 | G    |
| 40  | a     | 1816 | C    |
| 40  | a     | 1829 | A    |
| 40  | a     | 1833 | C    |
| 40  | a     | 1847 | A    |
| 40  | a     | 1848 | A    |
| 40  | a     | 1858 | A    |
| 40  | a     | 1859 | U    |
| 40  | a     | 1862 | G    |
| 40  | a     | 1864 | U    |
| 40  | a     | 1869 | G    |
| 40  | a     | 1870 | C    |
| 40  | a     | 1872 | A    |
| 40  | a     | 1873 | G    |
| 40  | a     | 1905 | C    |
| 40  | a     | 1906 | G    |
| 40  | a     | 1907 | G    |
| 40  | a     | 1913 | A    |
| 40  | a     | 1914 | C    |
| 40  | a     | 1919 | A    |
| 40  | a     | 1920 | C    |
| 40  | a     | 1922 | G    |
| 40  | a     | 1923 | U    |
| 40  | a     | 1924 | C    |
| 40  | a     | 1925 | C    |
| 40  | a     | 1926 | U    |
| 40  | a     | 1928 | A    |
| 40  | a     | 1929 | G    |
| 40  | a     | 1930 | G    |
| 40  | a     | 1936 | A    |
| 40  | a     | 1938 | A    |
| 40  | a     | 1955 | U    |
| 40  | a     | 1965 | C    |
| 40  | a     | 1967 | C    |
| 40  | a     | 1970 | A    |
| 40  | a     | 1971 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 1972 | G    |
| 40  | a     | 1987 | A    |
| 40  | a     | 1991 | U    |
| 40  | a     | 1992 | G    |
| 40  | a     | 1993 | U    |
| 40  | a     | 1997 | C    |
| 40  | a     | 2002 | G    |
| 40  | a     | 2022 | U    |
| 40  | a     | 2023 | C    |
| 40  | a     | 2027 | G    |
| 40  | a     | 2033 | A    |
| 40  | a     | 2043 | C    |
| 40  | a     | 2051 | A    |
| 40  | a     | 2052 | A    |
| 40  | a     | 2055 | C    |
| 40  | a     | 2056 | G    |
| 40  | a     | 2060 | A    |
| 40  | a     | 2061 | G    |
| 40  | a     | 2062 | A    |
| 40  | a     | 2063 | C    |
| 40  | a     | 2077 | A    |
| 40  | a     | 2097 | A    |
| 40  | a     | 2099 | U    |
| 40  | a     | 2100 | G    |
| 40  | a     | 2108 | A    |
| 40  | a     | 2110 | G    |
| 40  | a     | 2111 | U    |
| 40  | a     | 2113 | U    |
| 40  | a     | 2115 | G    |
| 40  | a     | 2116 | G    |
| 40  | a     | 2117 | A    |
| 40  | a     | 2118 | U    |
| 40  | a     | 2121 | G    |
| 40  | a     | 2122 | U    |
| 40  | a     | 2124 | G    |
| 40  | a     | 2125 | G    |
| 40  | a     | 2126 | A    |
| 40  | a     | 2127 | G    |
| 40  | a     | 2128 | G    |
| 40  | a     | 2131 | U    |
| 40  | a     | 2132 | U    |
| 40  | a     | 2133 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 2134 | A    |
| 40  | a     | 2139 | U    |
| 40  | a     | 2141 | G    |
| 40  | a     | 2146 | C    |
| 40  | a     | 2147 | A    |
| 40  | a     | 2154 | A    |
| 40  | a     | 2157 | G    |
| 40  | a     | 2158 | A    |
| 40  | a     | 2159 | G    |
| 40  | a     | 2162 | G    |
| 40  | a     | 2163 | A    |
| 40  | a     | 2164 | C    |
| 40  | a     | 2165 | C    |
| 40  | a     | 2169 | A    |
| 40  | a     | 2171 | A    |
| 40  | a     | 2172 | U    |
| 40  | a     | 2178 | C    |
| 40  | a     | 2182 | U    |
| 40  | a     | 2183 | A    |
| 40  | a     | 2185 | U    |
| 40  | a     | 2188 | U    |
| 40  | a     | 2189 | U    |
| 40  | a     | 2190 | G    |
| 40  | a     | 2191 | A    |
| 40  | a     | 2193 | G    |
| 40  | a     | 2194 | U    |
| 40  | a     | 2198 | A    |
| 40  | a     | 2204 | G    |
| 40  | a     | 2210 | U    |
| 40  | a     | 2211 | A    |
| 40  | a     | 2212 | A    |
| 40  | a     | 2213 | U    |
| 40  | a     | 2225 | A    |
| 40  | a     | 2226 | C    |
| 40  | a     | 2229 | U    |
| 40  | a     | 2238 | G    |
| 40  | a     | 2239 | G    |
| 40  | a     | 2244 | U    |
| 40  | a     | 2250 | G    |
| 40  | a     | 2268 | A    |
| 40  | a     | 2278 | A    |
| 40  | a     | 2283 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 2287 | A    |
| 40  | a     | 2297 | A    |
| 40  | a     | 2305 | U    |
| 40  | a     | 2308 | G    |
| 40  | a     | 2309 | A    |
| 40  | a     | 2315 | G    |
| 40  | a     | 2322 | A    |
| 40  | a     | 2325 | G    |
| 40  | a     | 2327 | A    |
| 40  | a     | 2333 | A    |
| 40  | a     | 2339 | C    |
| 40  | a     | 2345 | G    |
| 40  | a     | 2347 | C    |
| 40  | a     | 2350 | C    |
| 40  | a     | 2361 | G    |
| 40  | a     | 2372 | U    |
| 40  | a     | 2376 | A    |
| 40  | a     | 2383 | G    |
| 40  | a     | 2385 | C    |
| 40  | a     | 2402 | U    |
| 40  | a     | 2403 | C    |
| 40  | a     | 2406 | A    |
| 40  | a     | 2423 | U    |
| 40  | a     | 2424 | C    |
| 40  | a     | 2425 | A    |
| 40  | a     | 2426 | A    |
| 40  | a     | 2429 | G    |
| 40  | a     | 2430 | A    |
| 40  | a     | 2431 | U    |
| 40  | a     | 2434 | A    |
| 40  | a     | 2435 | A    |
| 40  | a     | 2441 | U    |
| 40  | a     | 2447 | G    |
| 40  | a     | 2448 | A    |
| 40  | a     | 2470 | G    |
| 40  | a     | 2474 | U    |
| 40  | a     | 2476 | A    |
| 40  | a     | 2478 | A    |
| 40  | a     | 2484 | G    |
| 40  | a     | 2491 | U    |
| 40  | a     | 2502 | G    |
| 40  | a     | 2506 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 2507 | C    |
| 40  | a     | 2512 | C    |
| 40  | a     | 2513 | A    |
| 40  | a     | 2518 | A    |
| 40  | a     | 2520 | C    |
| 40  | a     | 2525 | G    |
| 40  | a     | 2529 | G    |
| 40  | a     | 2535 | G    |
| 40  | a     | 2547 | A    |
| 40  | a     | 2554 | U    |
| 40  | a     | 2566 | A    |
| 40  | a     | 2567 | G    |
| 40  | a     | 2572 | A    |
| 40  | a     | 2573 | C    |
| 40  | a     | 2574 | G    |
| 40  | a     | 2585 | U    |
| 40  | a     | 2586 | U    |
| 40  | a     | 2602 | A    |
| 40  | a     | 2603 | G    |
| 40  | a     | 2609 | U    |
| 40  | a     | 2610 | C    |
| 40  | a     | 2611 | C    |
| 40  | a     | 2613 | U    |
| 40  | a     | 2629 | U    |
| 40  | a     | 2663 | G    |
| 40  | a     | 2669 | G    |
| 40  | a     | 2671 | G    |
| 40  | a     | 2689 | U    |
| 40  | a     | 2690 | U    |
| 40  | a     | 2714 | G    |
| 40  | a     | 2722 | G    |
| 40  | a     | 2726 | A    |
| 40  | a     | 2744 | G    |
| 40  | a     | 2748 | A    |
| 40  | a     | 2757 | A    |
| 40  | a     | 2758 | A    |
| 40  | a     | 2765 | A    |
| 40  | a     | 2777 | G    |
| 40  | a     | 2778 | A    |
| 40  | a     | 2791 | G    |
| 40  | a     | 2793 | C    |
| 40  | a     | 2796 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | a     | 2797 | U    |
| 40  | a     | 2798 | U    |
| 40  | a     | 2799 | A    |
| 40  | a     | 2801 | G    |
| 40  | a     | 2818 | U    |
| 40  | a     | 2820 | A    |
| 40  | a     | 2823 | A    |
| 40  | a     | 2825 | G    |
| 40  | a     | 2849 | U    |
| 40  | a     | 2850 | A    |
| 40  | a     | 2859 | G    |
| 40  | a     | 2861 | U    |
| 40  | a     | 2867 | G    |
| 40  | a     | 2880 | C    |
| 40  | a     | 2884 | U    |
| 40  | a     | 2885 | G    |
| 40  | a     | 2891 | U    |
| 40  | a     | 2902 | C    |
| 43  | d     | 2    | G    |
| 43  | d     | 9    | G    |
| 43  | d     | 13   | G    |
| 43  | d     | 16   | G    |
| 43  | d     | 17   | C    |
| 43  | d     | 35   | C    |
| 43  | d     | 36   | C    |
| 43  | d     | 45   | A    |
| 43  | d     | 51   | G    |
| 43  | d     | 56   | G    |
| 43  | d     | 64   | G    |
| 43  | d     | 66   | A    |
| 43  | d     | 88   | C    |
| 43  | d     | 89   | U    |
| 43  | d     | 90   | C    |
| 43  | d     | 99   | A    |
| 43  | d     | 109  | A    |

All (52) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 7     | -17 | U    |
| 8   | 7     | -14 | U    |
| 8   | 7     | -11 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 7     | -3   | U    |
| 8   | 7     | 11   | U    |
| 10  | A     | 6    | G    |
| 10  | A     | 7    | G    |
| 10  | A     | 9    | G    |
| 10  | A     | 22   | G    |
| 10  | A     | 60   | U    |
| 10  | A     | 70   | G    |
| 10  | B     | 6    | G    |
| 10  | B     | 7    | G    |
| 10  | B     | 9    | G    |
| 10  | B     | 22   | G    |
| 10  | B     | 37   | A    |
| 10  | B     | 60   | U    |
| 17  | D     | 7    | A    |
| 17  | D     | 70   | U    |
| 17  | D     | 121  | U    |
| 17  | D     | 181  | A    |
| 17  | D     | 183  | C    |
| 17  | D     | 197  | A    |
| 17  | D     | 209  | U    |
| 17  | D     | 305  | G    |
| 17  | D     | 328  | C    |
| 17  | D     | 428  | G    |
| 17  | D     | 496  | A    |
| 17  | D     | 517  | G    |
| 17  | D     | 531  | U    |
| 17  | D     | 532  | A    |
| 17  | D     | 562  | U    |
| 17  | D     | 641  | U    |
| 17  | D     | 722  | G    |
| 17  | D     | 793  | U    |
| 17  | D     | 991  | U    |
| 17  | D     | 992  | U    |
| 17  | D     | 1109 | C    |
| 17  | D     | 1145 | A    |
| 17  | D     | 1196 | A    |
| 17  | D     | 1211 | U    |
| 17  | D     | 1212 | U    |
| 17  | D     | 1213 | A    |
| 17  | D     | 1214 | C    |
| 17  | D     | 1225 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 17  | D     | 1299 | A    |
| 17  | D     | 1396 | A    |
| 17  | D     | 1432 | G    |
| 17  | D     | 1447 | A    |
| 17  | D     | 1491 | G    |
| 17  | D     | 1492 | A    |
| 17  | D     | 1493 | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

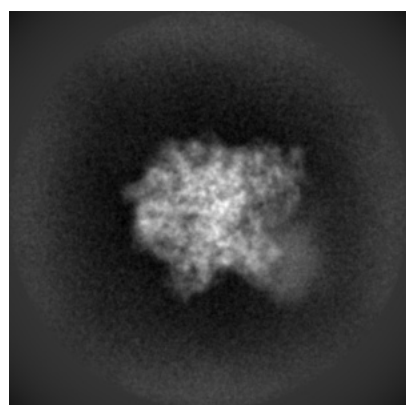
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22181. These allow visual inspection of the internal detail of the map and identification of artifacts.

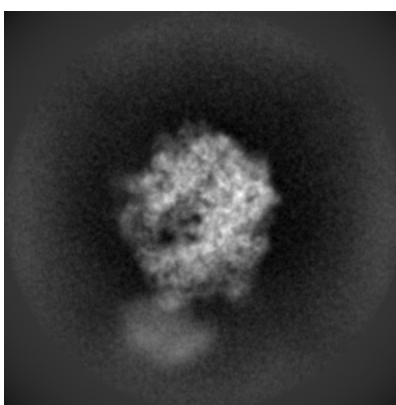
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

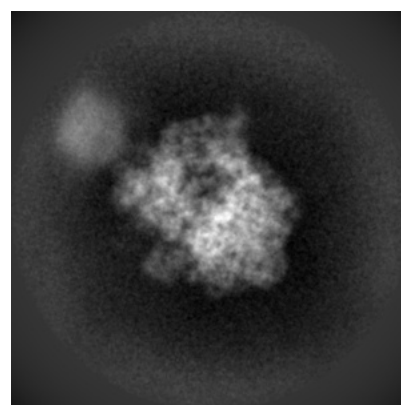
#### 6.1.1 Primary map



X



Y

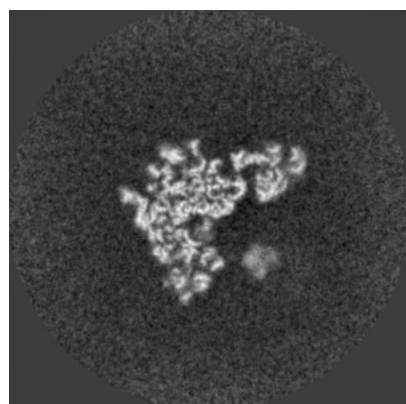


Z

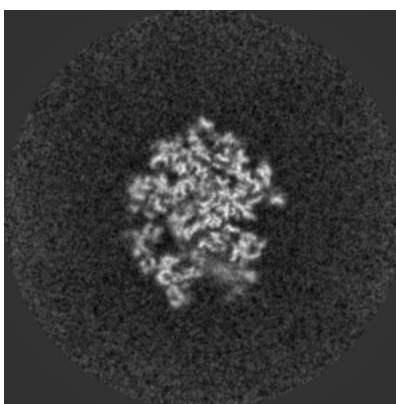
The images above show the map projected in three orthogonal directions.

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

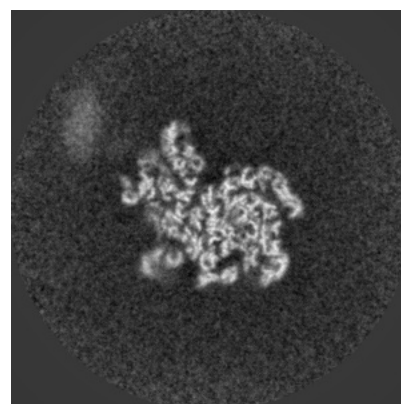
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

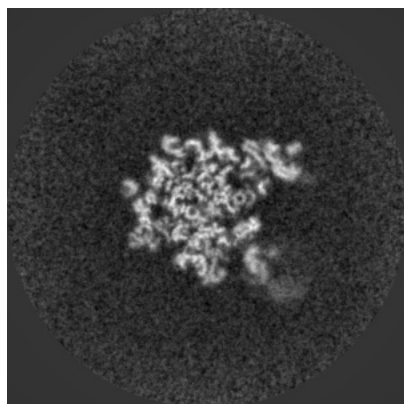


Z Index: 256

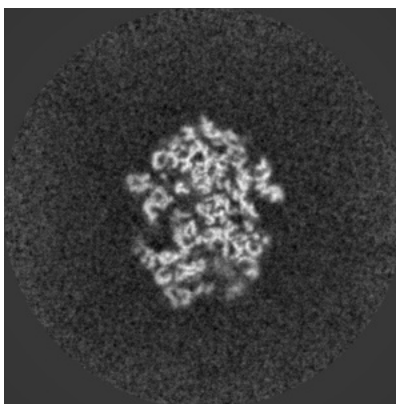
The images above show central slices of the map in three orthogonal directions.

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

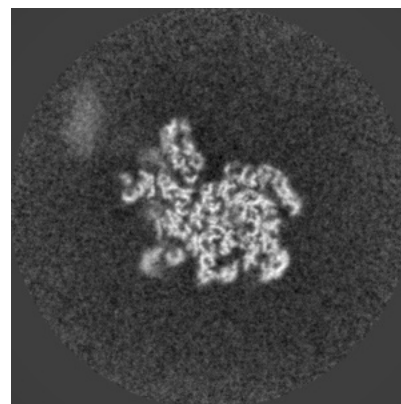
### 6.3.1 Primary map



X Index: 281



Y Index: 262

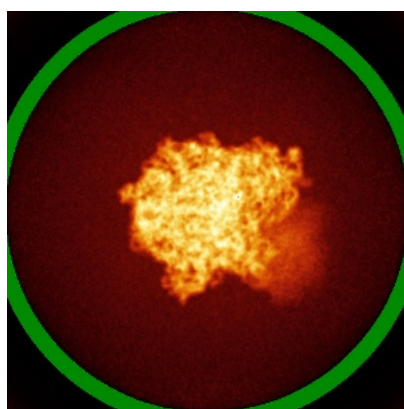


Z Index: 258

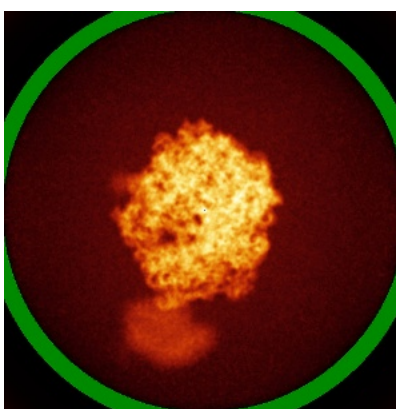
The images above show the largest variance slices of the map in three orthogonal directions.

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

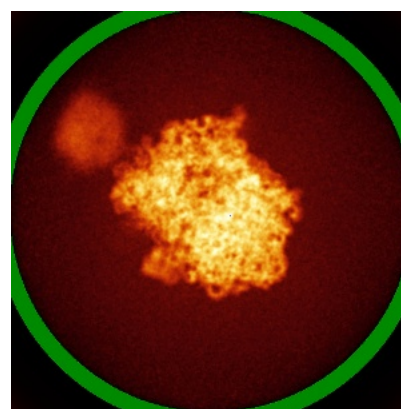
### 6.4.1 Primary map



X



Y

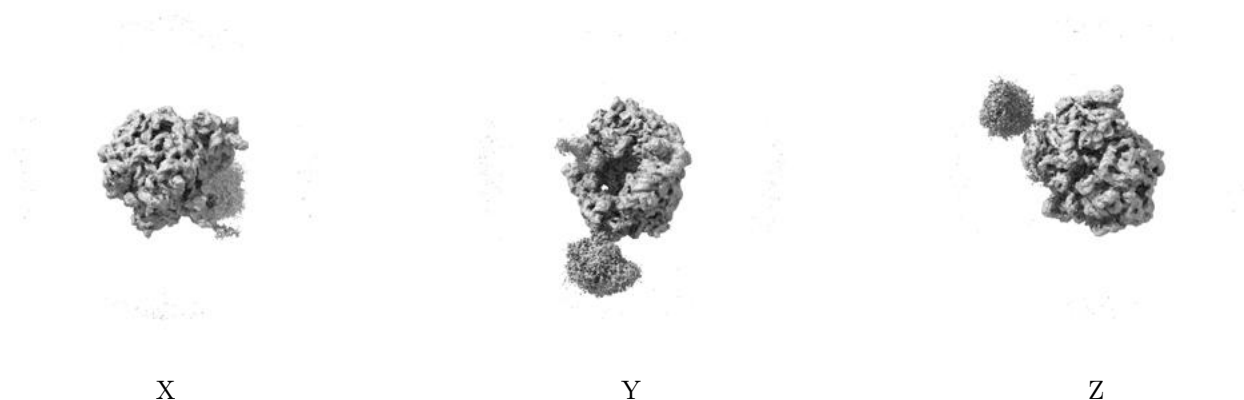


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0062. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

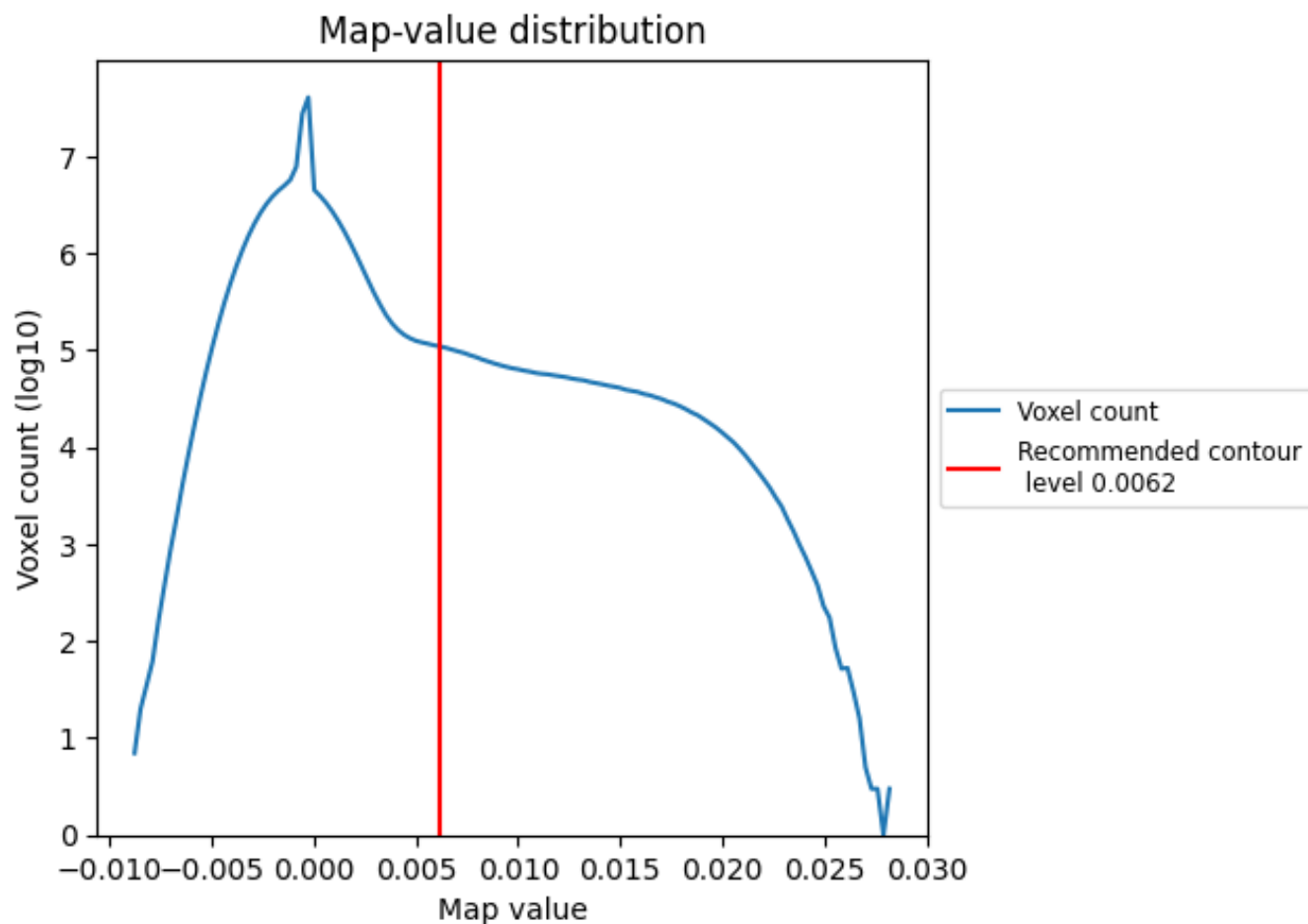
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

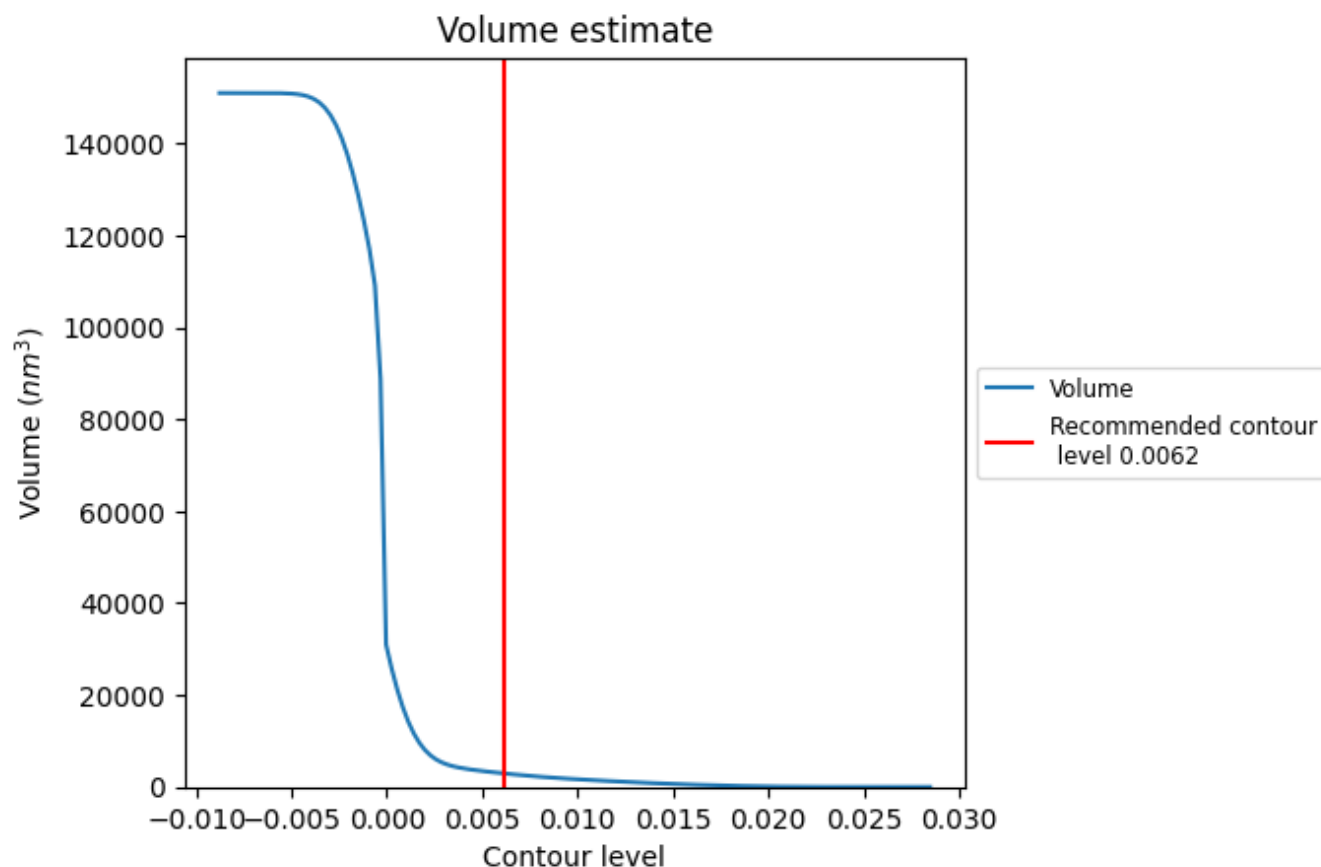
This section contains the results of statistical analysis of the map.

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



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

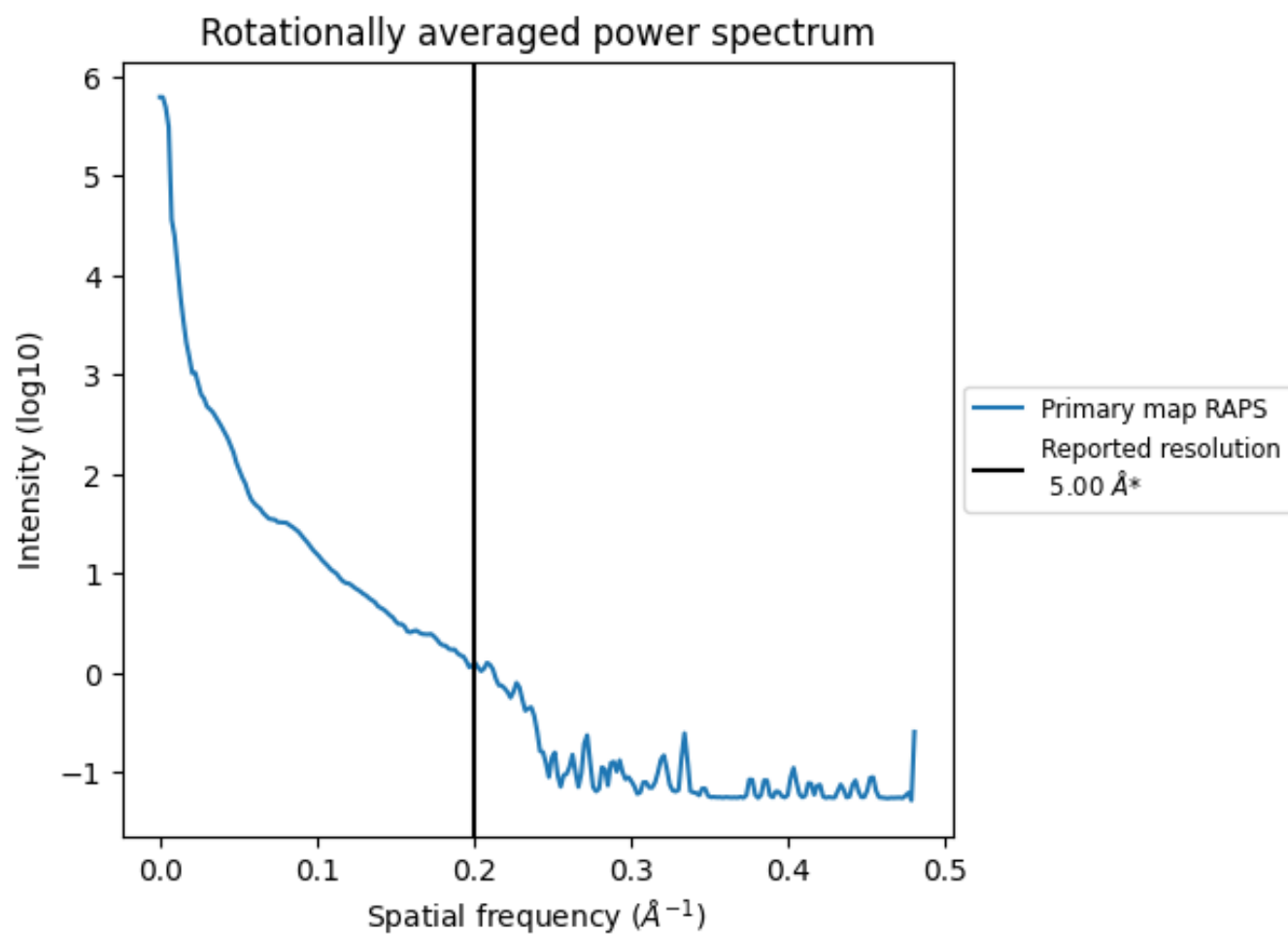
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2918  $\text{nm}^3$ ; this corresponds to an approximate mass of 2636 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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.200 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

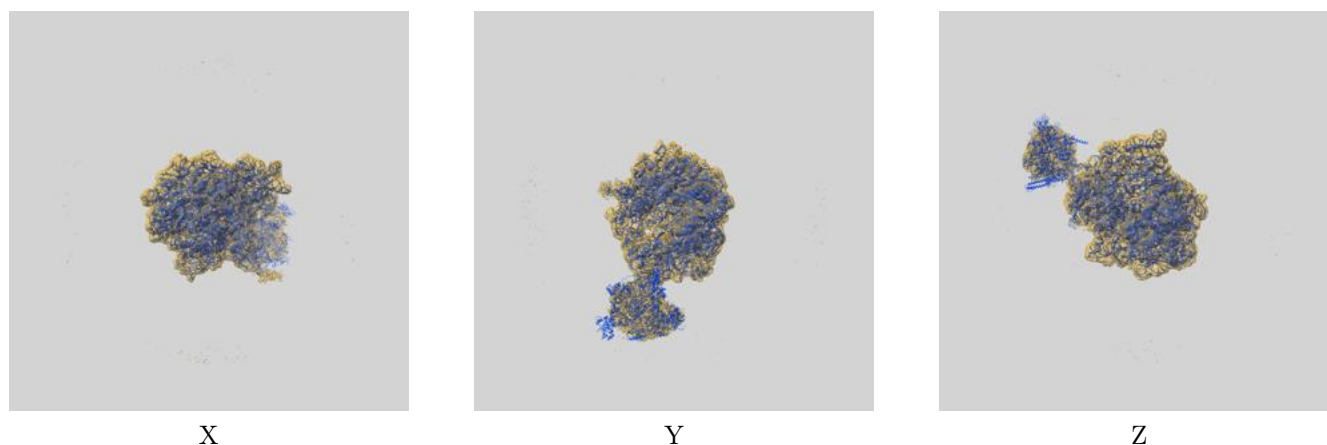
This section was not generated. No FSC curve or half-maps provided.



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

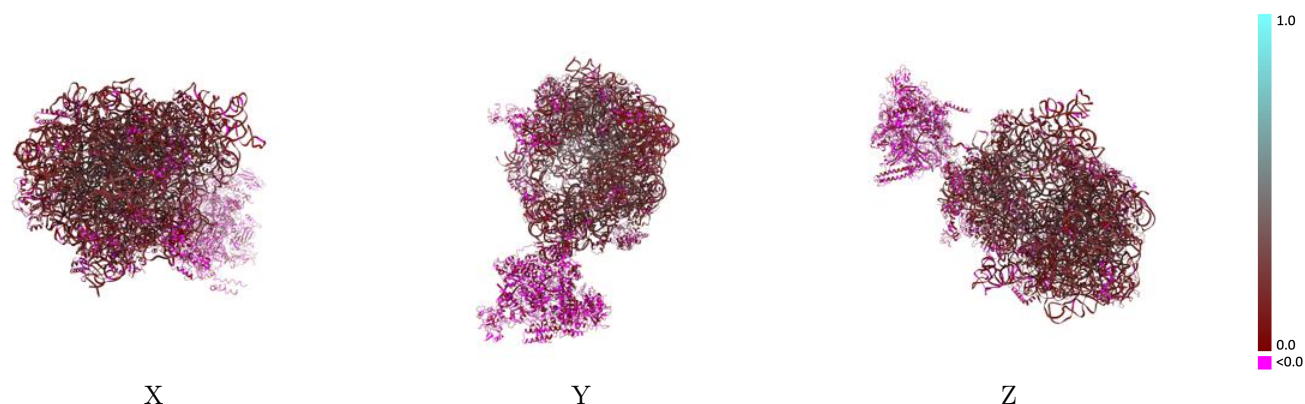
This section contains information regarding the fit between EMDB map EMD-22181 and PDB model 6XGF. Per-residue inclusion information can be found in section 3 on page 17.

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



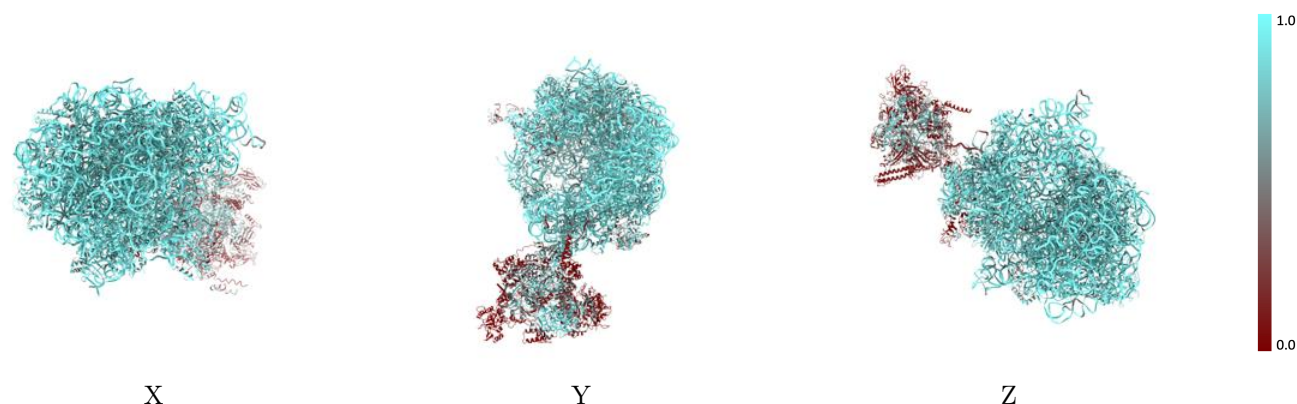
The images above show the 3D surface view of the map at the recommended contour level 0.0062 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



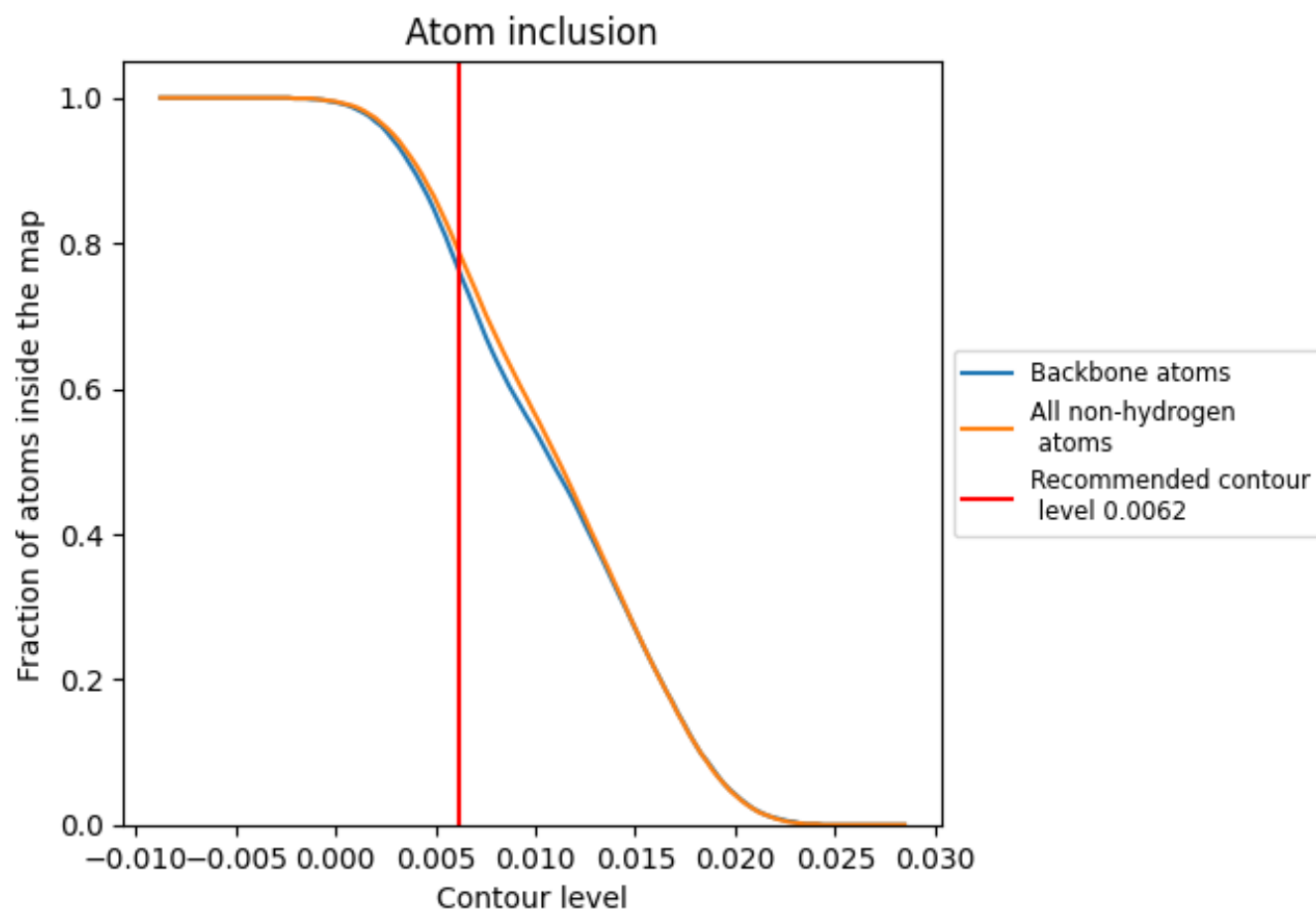
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0062).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 79% 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 (0.0062) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7860   |  0.1570   |
| 0     |  0.8470   |  0.1330   |
| 1     |  0.8340   |  0.2010   |
| 2     |  0.8210   |  0.1200   |
| 3     |  0.8420   |  0.1000   |
| 4     |  0.8670   |  0.1150   |
| 5     |  0.4910   |  0.0080   |
| 6     |  0.6200   |  0.0410   |
| 7     |  0.5930   |  0.0740   |
| 9     |  0.6710   |  0.0440   |
| A     |  0.9220   |  0.1560   |
| AA    |  0.4420   |  0.0190   |
| AB    |  0.2320   |  0.0300   |
| AC    |  0.2490   |  0.0050   |
| AD    |  0.1480  |  0.0140  |
| AE    |  0.3760 |  0.0230 |
| AF    |  0.1040 |  0.0020 |
| B     |  0.7560 |  0.0840 |
| C     |  0.8340 |  0.1330 |
| D     |  0.9700 |  0.2210 |
| E     |  0.8550 |  0.1270 |
| F     |  0.7550 |  0.1790 |
| G     |  0.8110 |  0.1430 |
| H     |  0.3310 |  0.0420 |
| I     |  0.7940 |  0.1620 |
| J     |  0.8470 |  0.1360 |
| K     |  0.8700 |  0.2170 |
| L     |  0.8270 |  0.1170 |
| M     |  0.8060 |  0.1440 |
| N     |  0.8440 |  0.1680 |
| O     |  0.8460 |  0.1000 |
| P     |  0.7520 |  0.1010 |
| Q     |  0.8480 |  0.1560 |
| R     |  0.8550 |  0.2250 |
| S     |  0.8450 |  0.1030 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| T     |  0.8550   |  0.1540   |
| U     |  0.8630   |  0.1180   |
| V     |  0.8280   |  0.1610   |
| W     |  0.7330   |  0.0620   |
| X     |  0.7630   |  0.0950   |
| Y     |  0.5330   |  0.0390   |
| Z     |  0.3520   |  0.0080   |
| a     |  0.9630   |  0.2100   |
| b     |  0.8480   |  0.1160   |
| c     |  0.8440   |  0.1670   |
| d     |  0.9580   |  0.1560   |
| e     |  0.8360   |  0.0720   |
| f     |  0.8740   |  0.1530   |
| g     |  0.7100   |  0.0580   |
| h     |  0.8790   |  0.1660   |
| i     |  0.8670   |  0.1790   |
| j     |  0.8500   |  0.1300   |
| k     |  0.7890   |  0.1000   |
| l     |  0.8160   |  0.1340   |
| m     |  0.8960  |  0.2070  |
| n     |  0.8250 |  0.0880 |
| o     |  0.8090 |  0.1430 |
| p     |  0.8330 |  0.0810 |
| q     |  0.8460 |  0.0900 |
| r     |  0.6570 |  0.0880 |
| s     |  0.8600 |  0.1280 |
| t     |  0.7770 |  0.1410 |
| u     |  0.8360 |  0.1480 |
| v     |  0.8450 |  0.1540 |
| w     |  0.8580 |  0.1390 |
| x     |  0.8920 |  0.0530 |
| y     |  0.8190 |  0.1110 |
| z     |  0.8960 |  0.1610 |